Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

Figure 1: HIV-1 gp41 Structure and Peptides

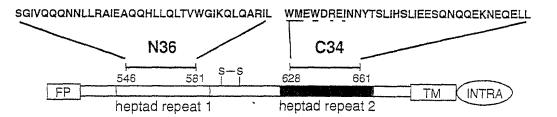
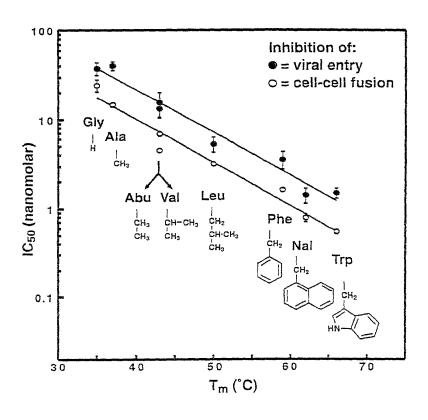


Figure 2: Correlation of C34 Inhibitory Potency With N36/C34 Stability



Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion

Inventors: Debra M. Eckert, et al.

Figure 3: D-peptide Sequences

D10pep1: Ac-GACEARHREWAWLCAA-CONH2
D10pep1a: Ac-KKGACEARHREWAWLCAA-CONH2

D10pep3: Ac - KK G A C G L G Q E E W F W L C A A - CONH2

D10pep4: Ac - GACDLKAKEWFWLCAA - CONH2

D10pep5: Ac - KK G A C E L L G W E W A W L C A A - CONH2
D10pep5a: Ac - KKKK G A C E L L G W E W A W L C A A - CONH2

D10pep6 : Ac - G A C S R S Q P E W E W L C A A - CONH2
D10pep6a : Ac - KK G A C S R S Q P E W E W L C A A - CONH2

D10pep7a: Ac - KK G A C L L R A P E W G W L C A A - CONH2

D10pep10: Ac - KK G A C M R G E W E W S W L C A A - CONH2

D10pep12: Ac - K K G A C P P L N K E W A W L C A A - CONH2

Consensus Sequence

CXXXXXEWXWLC

#### Where:

G = glycine

A = alanine

C = cysteine

D = aspartic acid

L = leucine

K = lysine

E = glutamic acid

W = tryptophan

F = phenylalanine

R = arginine

H = histidine

S = serine

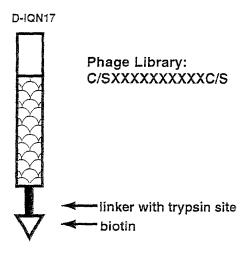
Q = glutamine

Docket/App No.: 0399.1192-008

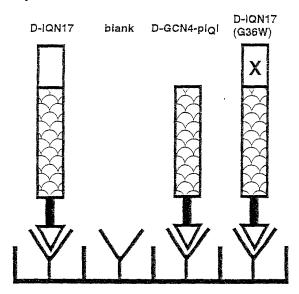
Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

Figure 4: Mirror-Image Phage Display with the D-IQN17 Target

1. Perform rounds of phage selection to identify binders to D-IQN17.

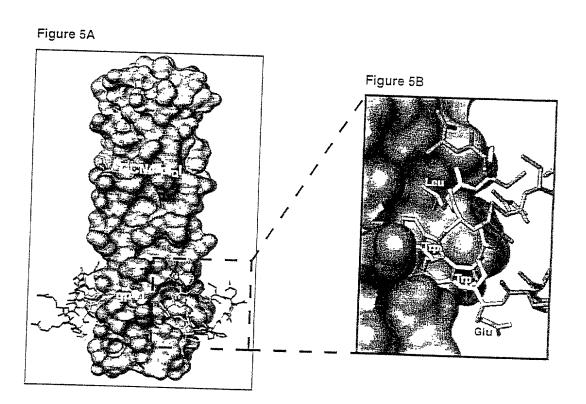


- 2. Sequence individual phage clones
- 3. Test for specificity of binding. Determine if the phage bind to the gp41 region of D-IQN17.



- 4. Synthesize D-peptides.
- 5. Assay anti-HIV activity of D-peptides.

# Relationship of D-peptides to IQN17



Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

Inventors:

Debra M. Eckert, et al.

#### Syncytia Assays

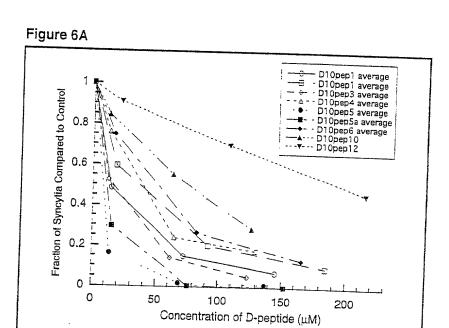


Figure 6B: IC<sub>50</sub> Data for D-Peptides:

D-Peptide	Approximate IC <sub>50</sub> Value (from one or more experiments)
D10pep1	2 x 10 <sup>-5</sup> M
D10pep1A	3 x 10 <sup>-5</sup> M
D10pep3	1 x 10 <sup>-5</sup> M
D10pep4	3 x 10 <sup>-5</sup> M
D10pep5	3 x 10 <sup>-6</sup> M
D10pep5a	6 x 10 <sup>-6</sup> M
D10pep6	4 x 10 <sup>-5</sup> M
D10pep7a	6 x 10 <sup>-5</sup> M
Dpep10	6 x 10 <sup>-5</sup> M
Dpep12	2 x 10 <sup>-4</sup> M

show anti-viral effects with  $IC_{50}$  values of less than 1 x  $10^{-4}$  M. D10pep3 D10pep4 D10pep5

```
REMARK
          3
 REMARK
          3 REFINEMENT.
 REMARK
               PROGRAM
                           : CNS 0.5
 REMARK
              AUTHORS
                           : BRUNGER, ADAMS, CLORE, DELANO,
 REMARK
                             GROS, GROSSE-KUNSTLEVE, JIANG,
 REMARK
                             KUSZEWSKI, NILGES, PANNU, READ,
 REMARK
                             RICE, SIMONSON, WARREN
 REMARK
 REMARK
          3 DATA USED IN REFINEMENT.
 REMARK
              RESOLUTION RANGE HIGH (ANGSTROMS) : 1.50
 REMARK
              RESOLUTION RANGE LOW (ANGSTROMS) :10.00
 REMARK
              DATA CUTOFF
         3
                                     (SIGMA(F)) : 0.0
 REMARK
              DATA CUTOFF HIGH
                                       (ABS(F)) :
                                                     646169.44
         3 DATA CUTOFF LOW
 REMARK
                                        (ABS(F)) :
                                                     0.000000
 REMARK
         3 COMPLETENESS (WORKING+TEST) (%): 94.6
 REMARK
              NUMBER OF REFLECTIONS
                                                 : 13549
 REMARK
 REMARK
         3 FIT TO DATA USED IN REFINEMENT.
 REMARK
          3
             CROSS-VALIDATION METHOD
                                                : THROUGHOUT
             FREE R VALUE TEST SET SELECTION : RANDOM
REMARK
REMARK
         3 R VALUE
                       (WORKING SET) : 0.214
         3 FREE R VALUE
3 FREE R VALUE TEST SET SIZE
REMARK
REMARK
                                           (%): 10.1
REMARK
         3 FREE R VALUE TEST SET COUNT
REMARK
         3
             ESTIMATED ERROR OF FREE R VALUE : 0.007
REMARK
         3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK
REMARK
         3 TOTAL NUMBER OF BINS USED
REMARK
             BIN RESOLUTION RANGE HIGH
                                               (A): 1.50
         3 BIN RESOLUTION RANGE LOW
REMARK
                                              (A): 1.59
REMARK
         3 BIN COMPLETENESS (WORKING+TEST) (%): 96.1
         REFLECTIONS IN BIN (WORKING SET): 2008
BIN R VALUE (WORKING SET): 0.233
REMARK
REMARK
REMARK
         3 BIN FREE R VALUE
                                                  : 0.270
         3 BIN FREE R VALUE TEST SET SIZE (%): 9.8
3 BIN FREE R VALUE TEST SET COUNT: 219
REMARK
REMARK
REMARK
         3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.018
REMARK
         3
REMARK
         3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK
         3 PROTEIN ATOMS
                                   :
REMARK
         3
             NUCLEIC ACID ATOMS
REMARK
             HETEROGEN ATOMS
                                            0
            SOLVENT ATOMS
REMARK
         3
REMARK
         3
REMARK
         3 B VALUES.
            FROM WILSON PLOT
REMARK
         3
                                       (A**2) : 21.6
REMARK
         3
             MEAN B VALUE (OVERALL, A**2) : 29.7
REMARK
             OVERALL ANISOTROPIC B VALUE.
         3
REMARK
              B11 (A**2) : 3.61
B22 (A**2) : 3.61
REMARK
         3
             B33 (A**2) : -7.22
B12 (A**2) : 1.74
B13 (A**2) : 0.00
REMARK
         3
REMARK
         3
REMARK
             B23 (A**2) : 0.00
REMARK
REMARK
REMARK
            BULK SOLVENT MODELING.
             METHOD USED : FLAT MODEL
REMARK
         3
REMARK
             KSOL
                         : 0.394054
```

Figure 7A

```
REMARK
       3 ESOL
                   : 58.3445 (A**2)
 REMARK
 REMARK
        3 ESTIMATED COORDINATE ERROR.
         ESD FROM LUZZATI PLOT
 REMARK
                                 (A) : 0.18
 REMARK
        3
          ESD FROM SIGMAA
                                 (A): 0.09
 REMARK
        3
          LOW RESOLUTION CUTOFF
                                 (A): 5.00
 REMARK
 REMARK
        3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
 REMARK
          ESD FROM C-V LUZZATI PLOT
                               (A): 0.20
 REMARK
          ESD FROM C-V SIGMAA
                                 (A) : 0.12
 REMARK
        3 RMS DEVIATIONS FROM IDEAL VALUES.
 REMARK
 REMARK
          BOND LENGTHS
                                (A): 0.012
 REMARK
          BOND ANGLES
                            (DEGREES) : 1.5
          DIHEDRAL ANGLES
 REMARK
        3
                            (DEGREES) : 15.7
 REMARK
        3
          IMPROPER ANGLES
                            (DEGREES) : 1.00
 REMARK
 REMARK
       3 ISOTROPIC THERMAL MODEL : RESTRAINED
 REMARK
REMARK
       3 ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                        RMS
                                             SIGMA
 REMARK
       3 MAIN-CHAIN BOND
                                (A**2) : 0.956 ; 2.0
REMARK
          MAIN-CHAIN ANGLE
       3
                                 (A**2) : 1.503 ; 3.0
REMARK
       3
          SIDE-CHAIN BOND
                                (A**2) : 1.853 ; 3.0
REMARK
         SIDE-CHAIN ANGLE
                                (A**2) : 2.676
REMARK
REMARK
       3 NCS MODEL : NONE
REMARK
      3 NCS RESTRAINTS.
3 GROUP
REMARK
                                       RMS
                                           SIGMA/WEIGHT
         GROUP 1 POSITIONAL GROUP 1 B-FACTOR
REMARK
                                (A) : NULL ; NULL
REMARK
                                (A**2) : NULL ; NULL
      3
3 PARAMETER FILE 1 : protein_rep_d.param
3 PARAMETER FILE 2 : CNS_TOPPAR/water_rep.param
REMARK
REMARK
REMARK
REMARK
      3 PARAMETER FILE 3 : CNS_TOPPAR/ion.param
      3 TOPOLOGY FILE 1 : CNS_TOPPAR/protein.top
3 TOPOLOGY FILE 2 : CNS_TOPPAR/water.top
REMARK
REMARK
      3 TOPOLOGY FILE 2 : CNS_TOPPAR/water.top
3 TOPOLOGY FILE 3 : CNS_TOPPAR/ion.top
REMARK
REMARK
REMARK
      3 OTHER REFINEMENT REMARKS: NULL
SEQRES
      1 A 214 ACE ARG MET LYS GLN ILE GLU ASP LYS ILE GLU GLU ILE
SEQRES
       2 A 214 GLU SER LYS GLN LYS LYS ILE GLU ASN GLU ILE ALA ARG
SEQRES
       3 A 214 ILE LYS LYS LEU LEU GLN LEU THR VAL TRP GLY ILE LYS
SEQRES
      4 A 214 GLN LEU GLN ALA ARG ILE LEU ACE DLY DLA DCS DLU DLA
SEQRES
       5 A 214 DRG DIS DRG DLU DRP DLA DRP DEU DCS DLA DLA CL WAT
          SEQRES
      бА
SEQRES
      SEQRES
      SEQRES
       9 A
           SEORES
      SEQRES
SEQRES 17 A 214 WAT WAT WAT WAT WAT CRYST1 41.829 41.829 84.817 90.00 90.00 120.00 P 3 2 1
ORIGXI
         1.000000 0.000000 0.000000
                                  0.00000
```

Figure 7B

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ORIGX2		0.0	0000	n	1.000000	0.0000	000	0 0000	0	
ORIGX3			0000		0.000000			0.0000		
SCALE1								0.0000		
			2390		0.013803			0.0000	0	
SCALE2			0000		0.027605			0.0000	0	
SCALE3			0000	0	0.000000	0.0117		0.0000	0	
ATOM	7	CA	. AC	ΕA	0	26 830	7.813	-22.925	1.00 54.89	A
ATOM	2	С	AC.	ΕA	0	26.773		-22.017		
ATOM	3		AC	ΞA	ō	25.855		-22.124		A
ATOM	4			G A		27.749			1.00 54.90	A
ATOM	5						9.141	-21.117	1.00 54.75	A
				G A	1	27.815		-20.165	1.00 54.58	A
ATOM	5			G A	1	27.625		-20.887	1.00 54.54	A
ATOM	7		AR	G A	1	27.841	12.790	-20.010	1.00 54.10	A
ATOM	8	CD	AR(	3 A	1	27.657	14.085	-20.800	1.00 54.18	A
ATOM	9	NΞ	AR	G A	1	28.177		-20.086	1.00 54.02	
ATOM	10	CZ	AR	3 A	1	29.470		-19.870		A
ATOM	11	MH	1 AR		1	30.395			1.00 54.03	A
ATOM	12		2 AR			29.843		-20.312	1.00 53.79	A
ATOM	13				1			-19.206	1.00 53.77	A
		C		3 A	1	26.752		-19.074	1.00 54.54	Ą
ATOM	14	0		3 A	1	27.042	10.224	-17.884	1.00 54.51	A
MOTA	15	N	ME:	ΓА	2	25.518	9.809	-19.480	1.00 54.42	A
ATOM	16	CA	MET	r A	2	24.445		-18.515	1.00 54.44	A
ATOM	17	CB	MET	Α 1	2	23.074	9 796	-19,202	1.00 54.68	
ATOM	18	CG	MET		2	22.749		-20.238		A
ATOM	19	SD	MET		2	21.345			1.00 54.76	A
ATOM	20	CE						-21.275	1.00 55.63	A
			MET		2	22.189		-22.822	1.00 55.29	A
ATOM	21	С	MET		2	24.557		-17.755	1.00 54.51	A
ATOM	22	0	MET	A	2	24.073	8.249	-16.629	1.00 54.42	A
ATOM	23	N	LYS	A	3	25.208		-18.362	1.00 54.34	A
ATOM '	24	CA	LYS	A	3	25.383		-17,702	1.00 54.29	
ATOM	25	CB	LYS	A	3	26.212		-18.581		A
ATOM	26	CG	LYS		3	26.527			1.00 54.05	A
ATOM	27	CD	LYS		3			-17.956	1.00 54.04	A
ATOM	28					27.727		-17.018	1.00 54.12	A
		CE	LYS		3	28.108		-16.513	1.00 54.37	A
ATOM	29	NZ	LYS		3	29.332	2.493	-15.656	1.00 53.92	A
ATOM	30	С	LYS	A	3	26.097	6.344	-16.384	1.00 54.33	A
ATOM	31	0	LYS	Α	3	25.779	5.740	-15.353	1.00 54.60	A
ATOM	32	N	GLN	A	4	27.064		-16.426	1.00 53.94	Ā
ATOM	33	CA	GLN	A	4	27.811		-15.236	1.00 53.69	
ATOM	34	CB	GLN		4	28.845		-15.580		A
ATOM	35	CG	GLN		4	29.861			1.00 54.21	A
ATOM	36	CD	GLN					-14.477	1.00 55.15	A
ATOM	37				4	29.621	10.285		1.00 55.56	A
			GLN		4	29.532	11.354 -		1.00 56.19	A
ATOM	38		GLN		4	29.533	10.209 -		1.00 55.66	A
ATOM	39	C	${\tt GLN}$	Α	4	26.828	8.182 -	-14.212	1.00 53,19	A
ATOM	40	0	${\tt GLN}$	A	4	26.972	7.953 -		1.00 53.10	A
ATOM	41	N	ILE	A	5	25.832	8.918 -		1.00 52.58	
ATOM	42	CA	ILE		5	24.817	9.523 -			A
ATOM	43	СЗ	ILE		5	23.826			1.00 51.70	A
ATOM	44	CG2					10.380 -		1.00 51.71	A
			ILE		5	22.643	10.812 -		1.00 51.41	A
ATOM	45		ILE		5	24.547	11.611 -		1.00 51.48	A
ATOM	46		ILE		5	23.646	12.569 -	16.017	1.00 51.33	A
ATOM	47	C	ILE	A	5	24.051	8.467 -		1.00 51.26	A
ATOM	48	0	ILE		5	23.650	8.700 -		1.00 51 09	
MOTA	49	N	GLU		6	23.864	7.300 -		1.00 50.54	A
MOTA	50	CA	GLU			23.146	6.214 -			A
ATOM	51	CB	GLU		6				1.00 50.01	A
ATOM	52	CG	GLU			22.789	5.148 ~		1.00 50.43	A
ATOM					6	22.141	5.721 -		1.00 51.26	A
AION	53	$\Box$	GLU	A.	5	22.045	4.703 -	15.400	1.00 51.68	A

Figure 7C

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

ATOM 54 OE1 GLU A 6 23.016 3.931 -16.557 1.00 52.29 55 OE2 GLU A 6 ATOM 4.682 -17.116 1.00 52.25 21.019 ATOM 23,995 5,606 -11.904 1.00 49.32 ATOM 57 0 GLU A 6 23.475 5.210 -10.859 1.00 49.24 7 ATOM 58 N ASP A 25.302 5.527 -12.128 1.00 48.32 CA ASP A 7 ATOM 59 26.178 4.970 -11.113 1.00 47.23 MOTA 60 CB ASP A 7 27.543 4.626 -11.703 1.00 47.92 ATOM 61 CG ASP A 7 27.450 3.585 -12.788 1.00 48.33 7 MOTA 62 OD1 ASP A 26.526 2.741 -12.729 1.00 48.43 MOTA 63 OD2 ASP A 7 28.310 3.606 -13.690 1.00 48.94 64 C 65 O ATOM ASP A 7 5.920 -9.926 1.00 46.09 26.344 7 5.481 -8.773 1.00 45.71 ATOM ASP A 26.283 Α 66 N LYS A 8 26.551 7.209 -10.201 1.00 44.57 MOTA 8 26.703 8 26.959 ATOM 67 CA LYS A 8.195 -9.129 1.00 43.01 9.598 -9.708 1.00 43.49 MOTA 68 CB LYS A 8 MOTA 69 CG LYS A 25.895 10.076 -10.695 1.00 44.78 26.423 8 8 70 CD LYS A 11.125 -11.702 1.00 45.38 ATOM ATOM 71 CE LYS A 26.698 12.490 -11.068 1.00 45.64 8 72 NZ LYS A ATOM 27.153 13.499 -12.069 1.00 45.55 73 C 74 O 8 25 413 8 25 419 8.171 -8.318 1.00 41.20 8.346 -7.098 1.00 40.61 ATOM LYS A MOTA LYS A 8 25.419 9 24.302 Α MOTA 75 N ILE A 7.935 -9.002 1.00 39.40 76 CA ILE A 77 CB ILE A 9 7.859 -8.333 1.00 37.29 7.859 -9.358 1.00 37.14 MOTA 23.015 ATOM 78 CG2 ILE A 9 20.600 21.872 A ATOM 7.251 -8 759 1.00 37.06 9 9 9.303 -9.812 1.00 36.95 9.440 -11.066 1.00 36.89 21.53± 20.801 ATOM 79 CG1 ILE A 21.631 ATOM 80 CD1 ILE A A ATOM 81 C ILE A 9 22.927 6.638 -7.418 1.00 36.07 A 82 O ILE A 9 83 N GLU A 10 6.756 -6.292 1.00 34.70 5.478 -7.887 1.00 34.23 ATOM 9 22.450 ATOM 23.389 Α ATOM 84 CA GLU A 10 23.353 4.260 -7.074 1.00 33.04 A 85 CB GLU A 10 86 CG GLU A 10 3.013 -7.847 1.00 32.87 MOTA 23.884 MOTA 23.890 1.705 -6.991 1.00 33.10 -7.747 1.00 33.56 MOTA 87 CD GLU A 10 24.287 0.417 Α 88 OE1 GLU A 10 ATOM 24.327 0.442 -8.999 1.00 34.07 24.542 -0.630 -7.084 1.00 32.41 89 OE2 GLU A 10 ATOM 90 C GLU A 10 91 O GLU A 10 -5.878 1.00 32.53 ATOM 24.244 4.556 A ATOM 24.009 4.069 -4.779 1.00 32,14 92 N GLU A 11 ATOM 25.259 5.380 -6.100 1.00 31.82 ATOM 93 CA GLU A 11 26.165 5.731 -5.018 1.00 31.36 94 CB GLU A 11 95 CG GLU A 11 ATOM 27.409 6.445 -5.536 1.00 33.18 Α ATOM 28.358 6.833 -4.423 1.00 35.22 A ATOM 96 CD GLU A 11 29.105 5.643 -3.822 1.00 36.93 97 OE1 GLU A 11 98 OE2 GLU A 11 MOTA 28.488 4.580 ~3.575 1.00 38.03 30.322 5.774 -3.579 1.00 38.85 MOTA GLU A 11 GLU A 11 ILE A 12 99 C 25.456 ATOM 6 621 -3.998 1.00 30.15 ATOM 100 0 25.556 6.377 -2.798 1.00 28.89 24.737 7.640 -4.471 1.00 29.09 ATOM 101 N CA ILE A 12 CB ILE A 12 ATOM 102 8.533 24.317 -3.550 1.00 28.34 9.675 -4.325 ATOM 103 23.301 1.00 28.74 CG2 ILE A 12 ATOM 104 22.206 10.281 -3.501 1.00 28.70 CG1 ILE A 12 CD1 ILE A 12 ATOM 105 24.327 10.743 -4.701 1.00 28.84 ATOM 106 23.922 11.603 -5.890 1.00 29.69 MOTA 107 ILE A 12 22.985 7.725 -2.761 1.00 27.83 ILE A 12 GLU A 13 ATOM 108 0 22.802 7.948 -1.560 1.00 26.46 109 N MOTA 6.790 -3.423 1.00 27.40 22.312 110 CA GLU A 13 111 CB GLU A 13 MOTA 21.313 5.965 -2.762 1.00 26.92 ATOM 20.579 5.087 -3.805 1.00 28.34

Figure 7D

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM	112	CG	GL	U A	. 13	19.760	5.937	-4.810	1.00 29.72	A
MOTA	113	CD	GL.	U A	. 13	19.080	5.118	-5.900	1.00 31.77	A
MOTA	114	OE	1 GL	U A	. 13	19.671	4.107	-6.331	1.00 33.64	A
ATOM	115	OE	2 GL	JA	13	17.960	5.495	-6,327	1.00 32.24	A
ATOM	116	С	GL	J A	13	31.975		-1.678	1.00 26.36	A
MOTA	117	0	GLI	J A	13	21.411		-0.597	1.00 25.75	A
ATOM	118	N	SE	R A	14	23.179	4.629	-1.950	1.00 26.17	A
ATOM	119	CA	SEI	R A	14	23.899	3.792	-0.999	1.00 26.31	A
ATOM	120	CB	SEI	Q A	14	25.184	3.224	-1.625	1.00 26.71	A
ATOM	121	OG	SE	R A	14	25.954	2.470	-0.695	1.00 30.07	A
ATOM	122	C	SEI	? A	14	24.246	4.626	0.221	1.00 25.81	A
ATOM	123	0	SEI	R A		24.079	4.149	1.339	1.00 25.13	A
ATOM	124	N	LYS			24.753	5.840	0.009	1.00 24.70	A
ATOM	125	CA	LYS	5 A	15	25.091	6.713	1.151	1.00 25.41	Ā
ATOM	126	CB	LYS		15	25.805	7.971	0.672	1.00 26.20	A
ATOM	127	CG	LYS		15	27.256	7.762	0.285	1.00 29.07	
ATOM	128	CD	LYS		15	27.875	9.077	-0.220	1.00 30.97	A.
ATOM	129	CE	LYS		15	29.328	8.914	-0.603	1.00 32.08	A
ATOM	130	NZ	LYS		15	29.547	7.749	-1.502	1.00 34.63	A
ATOM	131	C	LYS		15	23.824	7.102	1.938		A
ATOM	132	ō	LYS		15	23.862	7.279	3.171	1.00 24.45	A
ATOM	133	N	GLN		16	22.708	7.254	1.247	1.00 24.50	A
ATOM	134	CA	GLN		16	21.450	7.586	1.904	1.00 24.12	A
ATOM	135	CB	GLN		16	20.396	7.815	0.834	1.00 23.82	A
ATOM	136	CG	GLN		16	19.229	8.643	1.232	1.00 25.71	A
ATOM	137	CD	GLN		16	18.543	9.230	0.004	1.00 29.64	A
ATOM	138	OE1			16	18.015	8.498	-0.817	1.00 32.26	A
ATOM	139	NE2			16	18.569	10.556	-0.135	1.00 34.89	A
ATOM	140	C	GLN		16	21.027	5.447	2.838	1.00 32.74	A
ATOM	142	õ	GLN		16	20.584	6.681	3.979	1.00 23.67	A
ATOM	142	N	LYS		17	21.160	5.214	2.365	1.00 22.84	A
ATOM	143	CA	LYS		17	20.798	4.057		1.00 22.83	A
ATOM	144	CB	LYS		17	20.738	2.756	3.179 2.357	1.00 22.59	A
ATOM	145	CG	LYS		17	20.340	1.539	3.055	1.00 22.86	A
ATOM	146	CD	LYS		17	18.837	1.539		1.00 26.69	A
ATOM	147	CE	LYS		17 17	18.177	0.837	2.932	1.00 29.27	A
ATOM	148	NZ	LYS		17	16.686	0.870	4.051	1.00 31.75	A
ATOM	149	C	LYS		17	21.718		3.940	1.00 34.25	A
ATOM	150	0	LYS		17	21.261	4.015 3.747	4.406	1.00 22.31	A
ATOM	151	N	LYS		18	23.001	4 306	5.515 4.223	1.00 21.02	A
ATOM	152	CA	LYS		18	23.909			1.00 21.81	A
ATOM	153	CB	LYS		18	25.348	4.302	5.374	1.00 21.74	A.
ATOM	154	CG	LYS		18	26.029	4.540	4.964	1.00 24.04	A
ATOM	155	CD	LYS		18		3.321	4.401	1.00 27.30	A
ATOM	156	CE	LYS		18	27.381	3.712	3.863	1.00 29.23	A
ATOM	157	NZ	LYS			27.972	2.592	3.025	1.00 30.50	A
ATOM	158	C	LYS		18	29.290	3.010	2.472	1.00 33.57	A
ATOM	159	0			18	23.500	5.376	6.378	1.00 20.62	A
ATOM	160	N	LYS		18	23.565	5.138	7.577	1.00 19.85	A
			ILE		19	23.062	6.531	5.887	1.00 19.99	A
ATOM	161	CA	ILE		19	22.655	7.636	6.762	1.00 19.98	A
MOTA	162 163	CB	ILE		19	22.406	8.926	5.914	1.00 20.09	A
ATOM					19	21.554	9.944	6.682	1.00 20.80	A
ATOM	164		ILE		19	23.756	9.499	5.464	1.00 21.49	A
ATOM	165		ILE		19	23.669	10.495	4.296	1.00 21.18	A
ATOM	166	C	ILE		19	21.400	7.221	7.517	1.00 20.44	A
ATOM	167	0	ILE	A.	19	21.282	7.452	8 735	1.00 20.23	A
ATOM	168	N	GLU		20	20.459	6.569	5.836	1.00 20.24	A
ATOM	169	CA	GLU	A	20	19.230	6.149	7.503	1.00 20.43	A

Figure 7E

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

Inventors: Debra M. Eckert, et al.

MCTA	170	CB	GL	U A	20	18.223	5.608	6.484	1.00 22.94	А
ATOM	171	CG	GL	υA	20	17.766	6.671	5.499		A
ATOM	172	CD	GL	υA	20	16.926	6.108	4.378	1.00 29.04	A
MOTA	173	OE	1 GL	J A	20	16.961	4.873	4.177	1.00 30.40	A
ATOM	174	OE:	GLT	UA	20	16.243	6.901	3.691	1.00 30,73	A
ATOM	175	С		J A	20	19.533	5.109	8.576	1.00 30.88	
ATOM	176	0		JA	20	18.917	5.127	9.645	1.00 20.23	A
ATOM	177	N		N A	21	20.478	4.220	8.321	1.00 20.23	A
ATOM	178	CA		N A	21	20.820	3.212	9.328	1.00 20.33	A
ATOM	179	CB		N A	21	21.694	2.117	8.720		A
ATOM	180	CG		V A	21	20.875			1.00 24.15	A
ATOM	181		L ASI		21		1.155	7.872	1.00 25.28	A
ATOM	182		ASI			19.676	0.980	8.099	1.00 28.26	A
ATOM	183	C IVD.		4 V	21	21.505	0.549	6.870	1.00 26.78	A
ATOM	184				21	21.500	3.854	10.527	1.00 21.75	A
		0		I A	21	21.269	3.444	11.674	1.00 21.80	A
MOTA	185	N		JA	22	22.335	4.853	10.274	1.00 20.99	A
ATOM	186	CA	GLU		22	23.007	5.548	11.369	1.00 20.36	A
ATOM	197	CB	GLU		22	24.059	6.516	10.825	1.00 22.89	A
ATOM	188	CG	GLU		22	24.914	7.169	11.901	1.00 25.86	A
ATOM	189	CD	GLU		22	25.515	6.170	12.882	1.00 27.97	A
ATOM	190	OE:			22	26.121	5.158	12.444	1.00 30.05	A
ATOM	191	OE2			22	25.376	6.411	14.118	1.00 31.29	A
MOTA	192	С	GLU		22	21.952	6.294	12.187	1.00 19.79	A
MOTA	193	0	GLU	JA	22	21.988	6.264	13.445	1.00 18.87	A
ATOM	194	N	ILE	. A	23	21.003	6.951	11.518	1.00 18.92	A
MOTA	195	CA	ILE		23	19.955	7 670	12.254	1.00 18.60	A
ATOM	196	CB	ILE	A	23	19.012	8.388	11.244	1.00 18.79	A
ATOM	197	CG2	ILE	A	23	17.672	8.764	11.880	1.00 20.11	A
ATOM	198	CG1	ILE	A	23	19.739	9.598	10.701	1.00 20.45	A
ATOM	199	CD1	ILE	A	23	19.060	10.223	9.539	1.00 22.51	A
ATOM	200	C	ILE	Α	23	19.163	6.687	13.118	1.00 19.09	A
MOTA	201	0	ILE	A	23	18.807	7.006	14.260	1.00 18.74	A
MOTA	202	N	ALA	A	24	18.903	5.479	12.617	1.00 18.44	A
ATOM	203	CA	ALA	A	24	18.153	4.517	13.420	1.00 18.86	A
ATOM	204	CB	ALA	A	24	17.824	3.257	12.573	1.00 19.39	A
ATOM	205	С	ALA	A	24	18.947	4.136	14.665	1.00 18.66	Ā
ATOM	206	0	ALA	A	24	18.343	3.966	15.757	1.00 19.32	Ā
ATOM	207	N	ARG	A	25	20.272	4.028	14.548	1.00 18.57	A
ATOM	208	CA	ARG		25	21.111	3.667	15.709	1.00 19.19	A
ATOM	209	CB	ARG		25	22.552	3.343	15.287	1.00 20.85	A A
ATOM	210	CG	ARG		25	22.674	1.959	14.627	1.00 23.87	
ATOM	211	CD	ARG		25	24.108	1.536	14.429	1.00 25.32	A
ATOM	212	NE	ARG		25	24.759	2.294	13.376	1.00 27.13	A
ATOM	213	CZ	ARG		25	24.672	2.019	12.075	1.00 27.13	A
MOTA	214		ARG		25	23.955	0.979	11.641	1.00 28.92	A
ATOM	215		ARG		25	25.296	2.806	11.214	1.00 27.79	A
ATOM	216	С	ARG		25	21.083	4.819	16.722	1.00 27.79	A
ATOM	217	0	ARG		25	20.942	4.592	17.940		A
MOTA	218	N	ILE		26	21.201	6.041	16.221	1.00 17.93	A
ATOM	219	CA	ILE		26				1.00 17.83	A
ATOM	220	CB	ILE		26	21.184 21.369	7.222	17.080	1.00 16.94	A
ATOM	221		ILE		26		8.479	16.225	1.00 17.99	A
ATOM	222		ILE		2 6 2 6	20.943	9.741	17.006	1.30 19.34	A
ATOM	223		ILE		26	22.821	8.537	15.796	1.00 19.88	A
ATOM	224	CDI	ILE		26 26	23.144 19.876	9.587	14.721	1.00 21.83	A
ATOM	225	0	ILE		26 26		7.301	17.857	1.00 18.02	A
ATOM	226	N	LYS			19.875	7.580	19.055	1.00 17.73	A
ATOM	227	CA	LYS		27	18.752	7.069	17.191	1.00 17.60	A
191 0111		CA	22	A	27	17.450	7.137	17.853	1.00 17.90	A

Figure 7F

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM	228	CB	LYS	A	27	16.330	6.994	16.805	1.00 19.01	A
ATOM	229	CG	LYS		27	16.266	8,210	15.876	1.00 22.27	A
ATOM	230	CD		A	27	15.275	7.984	14.711	1.00 24.03	A
ATOM	231	CE	LYS	Ā	27	13.860	7.664	15.161	1.00 24.41	A
ATOM	232	NZ	LYS	A	2~	13.173	8.848	15.714	1.00 27.04	A
ATOM	233	С	LYS	ř.	27	17.326	6.097	18.969	1.00 18.17	A
MOTA	234	0	LYS	Ä	27	16.767	6.388	20.013	1.00 18.33	A
ATOM	235	N	LYS	A	28	17.871	4.896	18.775	1.00 17.00	A
ATOM	236	CA	LYS	A	28	17.788	3.867	19.790	1.00 17.21	A
MCTA	237	CB	LYS		28	18.244	2.503	19.223	1.00 18.92	A
ATOM	238	CG	LYS	A	28	17.288	1.982	18.164	1.00 24.56	A
ATOM	239	CD	LYS		28	17.833	0.732	17.454	1.00 26.88	A
ATOM	240	CE	LYS		28	16.950	0.371	16.260	1.00 28.84	A
MOTA	241	NZ	LYS		28	17.284	-0.938	15.592	1.00 31.36	A
ATOM	242	C	LYS		28	18.618	4.257	21.016	1.00 17.36	A
ATOM	243	0	LYS		28	18.159	4.066	22.165	1.00 17.54	A
ATOM	244	N	LEU		29	19.794	4.835	20.793	1.00 16.84	A
ATOM	245	CA	LEU		29	20.642	5.234	21.913	1.00 16.41	A
ATOM	246	CB	LEU		29	22.077	5.529	21.453	1.00 16.26	A
ATOM	247	CG	LEU		29	23.050	6.048	22.515	1.00 16.76	Ā
ATOM	248		LEU		29	23.062	5.096	23.701	1.00 16.47	A
ATOM	249	CD2	LEU		29	24.450	6.201	21.885	1.00 17.67	A
ATOM	250	C	LEU		29	20.023	6.429	22.506	1.00 16.92	A
MOTA	251	0	LEU		29	20.027	6.503	23,859	1.00 16.36	Ā
ATOM	252	N	LEU		30	19.447	7.343	21.820	1.00 15.57	A
ATOM	253	CA	LEU		30	18.818	8.519	22.424	1.00 15.77	A
ATOM	254	CB	LEU		30	18.401	9.501	21.298	1.00 15.65	Ā
ATOM	255	CG	LEU		30	17.717	10.780	21.696	1.00 17.55	A
ATOM	256		LEU		30	18.557	11.504	32,722	1.00 16.71	A
ATOM	257		LEU		3 C	17.552	11.602	20.399	1.00 18.10	A
ATOM	258	C	LEU		30	17.659	8.067	23.288	1.00 16.42	A
ATOM	259	0		A	30	17.466	8.604	24.399	1.00 17.55	A
ATOM	250	N	GLN		31	16.903	7.053	22.862	1.00 16.79	A
MOTA	261	CA	GLN		31	15.816	6.564	23.692	1.00 18.13	A
ATOM	262	CB	GLN		31	14.945	5.593	22.886	1.00 21.45	A
ATOM	263	CG	GLN		31	14.119	6.358	21.834	1.00 24.92	A
ATOM	264	CD	GLN		31	13.196	7.437	22.424	1.00 26.81	A
ATOM	265		GLN		31	12.913	8.459	21.786	1.00 28.75	A
ATOM	266	NE2	GLN		31	12.713	7.207	23.648	1.00 29.86	A
ATOM	267	C	GLN		31	16.319	5.958	25.008	1.00 17.24	Ā
MOTA	268	0	GLN		31	15.655	6.092	26.038	1.00 17.79	A
ATOM	269	N	LEU		32	17.494	5,307	24 987	1.00 15.77	A
ATOM	270	CA		A	32	18.070	4.755	26.209	1.00 14.63	A
ATOM	271	CB	LEU		32	19.314	3.932	25.911	1.00 16.13	A
ATOM	272	CG		A	32	19.015	2.574	25.275	1.00 18.58	A
ATOM	273		LEU		32	20.291	1.961	24.770	1.00 20.70	A
ATOM	274		LEU		32	18.337	1.698	26.315	1.00 22.17	A
ATOM	275	C	LEU		32	18.449	5.895	27.140	1.00 13.68	Ā
ATOM	276	0	LEU		32	18.258	5.774	28.357	1.00 13.31	Ā
ATOM	277	N	THR		33	18.980	6.991	26.600	1.00 13.42	A
ATOM	278	CA	THR		33	19.348	8.081	27.500	1.00 12.96	A
ATOM	279	CB	THR		33	20.236	9.134	26.820	1.00 12.30	A
ATOM	280		THR		33	19.530	9.745	25.733	1.00 15.40	A
ATOM	281		THR		33	21.567	8.508	26.358	1.00 15.01	A
ATOM	282	C	THR		33	18.124	8.742	28.117	1.00 13.01	A A
ATOM	283	0	THR		33	18.159	9.169	29.285	1.00 12.67	A
ATOM	284	N	VAL		34	17.038	8.838	27.345	1.00 13.20	A A
ATOM	285	CA	VAL		34	15.804	9.410	27.863	1.00 13.20	A A
EFT OLT	202	سم	ىنىد ٧	~	J=2	x5.004	>.≒±∪	.,,,,,,,	±3.50	A

Figure 7G

MOTA	286	CB	VAL :	A 34	14.708	9.498	26.773	1.00 14.31	A
ATOM	287	CGl	VAL :	A 34	13.380	9.811	27.382	1.00 15.35	A
ATOM	288	CG2	VAL :	A 34	15.096	10.517	25.710	1.00 15.04	A
ATOM	289	С	VAL	A 34	15.326	8.526	29.041	1.00 12.55	A
ATOM	290	0	VAL 2	34	14.997	9.016	30.131	1.00 13.43	A
ATOM	291	N	TRP 2	A 35	15.354	7.210	28.857	1.00 13.04	A
MOTA	292	CA	TRP .	A 35	14.946	6.289	29.908	1.00 13.11	A
MOTA	293	CB	TRP 2	A 35	14.988	4.861	29.319	1.00 14.19	A
ATOM	294	CG	TRP 2	A 35	14.672	3.785	30.334	1.00 15.43	A
ATOM	295	CD2	TRP A	A 35	15.610	3.101	31.191	1.00 15.26	A
ATOM	296	CE2	TRP :	A 35	14.860	2.165	31.963	1.00 15.57	A
ATOM	297	CE3	TRP 2	A 35	16.990	3.196	31.393	1.00 15.49	A
MOTA	298	CD1	TRP A	A 35	13.454	3.258	30.609	1.00 17.15	A
ATOM	299	NE1	TRP 2	A 35	13.553	2.281	31.572	1.00 17.80	A
ATOM	300	CZ2	TRP :	A 35	15.459	1.324	32.905	1.00 15.31	A
ATOM	301	CZ3	TRP I	A 35	17.600	2.355	32.349	1.00 16.17	A
ATOM	302			A 35	16.815	1.437	33.090	1.00 14.74	A
ATOM	303	C	TRP A		15.869	6.429	31.141	1.00 13.13	A
ATOM	304	0	TRP 2		15.418	6.409	32.278	1.00 12.76	A
ATOM	305	N	GLY 3		17.176	6.556	30.893	1.00 12.50	A
ATOM	306	CA	GLY A		18.118	6.668	31.998	1.00 12.50	A
ATOM	307	С	GLY A		17.887	7.936	32.817	1.00 11.58	A
ATOM	308	0	GLY A		17.917	7.875	34.042	1.00 11.70	A
ATOM	309	N	ILE A		17.656	9.084	32.174	1.00 11.85	A
MOTA	310	CA	ILE A		17.383	10.303	32.884	1.00 11.18	A
ATOM	311	CB		A 37	17.262	11.439	31.882	1.00 11.22	A
ATOM	312	CG2			16.680	12.660	32.600	1.00 13.25	A
ATOM	313	CG1			18.636	11.739	31.281	1.00 12.70	A
ATOM	314		ILE A		18.571	12.560	29.955	1.00 13.00	A
ATOM	315	C	ILE A	A 37	16.082	10.105	33.703	1.00 11.99	A
MOTA	316	0	ILE A	A 37	16.026	10.526	34.860	1.00 12.24	A
ATOM	317	N	LYS A		15.069	9.465	33.094	1.00 11.84	A
ATOM	318	CA	LYS A	38	13.825	9.215	33.809	1.00 13.62	A
ATOM	319	CB	LYS A	38	12.840	8.512	32.861	1.00 15.00	A
ATOM	320	CG	LYS A	A 38	11.429	8.437	33.369	1.00 17.76	A
MOTA	321	CD	LYS 2	A 38	10.545	7.835	32.247	1.00 20.78	A
MOTA	322	CE	LYS A		9.046	7.955	32.600	1.00 25.34	A
ATOM	323	NZ	LYS A		8.721	7.069	33.722	1.00 29.03	A
ATOM	324	С	LYS 2		14.060	8.399	35.083	1.00 12.64	A
ATOM	325	ō	LYS A		13,490	8.724	36.163	1.00 12.58	A
ATOM	326	N	GLN F		14.916	7 371	35.001	1.00 11.99	A
ATOM	327	CA	GLN A	A 39	15.176	6.573	36.189	1.00 11.84	A
MOTA	328	CB	GLN A	39	16.049	5.339	35.900	1.00 12.90	A
ATOM	329	CG	GLN A	39	15.580	4.440	34.757	1.00 14.71	A
ATOM	330	CD	GLN A	3 9	14.118	4.213	34.747	1.00 17.73	A
ATOM	331	OE1	GLN A	A 39	13.596	3.581	35.669	1.00 22.45	A
ATOM	332	NE2	GLN F	39	13.420	4.701	33.701	1.00 20.02	A
MOTA	333	C	GLN A	39	15.907	7.372	37.259	1.00 12.24	A
ATOM	334	0	GLN A	39	15.601	7.271	38.453	1.00 12.42	A
ATOM	335	N	LEU A	40	16.883	8.195	36.854	1.00 10.89	A
MOTA	336	CA	LEU A	4.0	17.632	8.980	37.853	1.00 11.44	A
ATOM	337	CB	LEU A		18.860	9.648	37.198	1.00 12.26	A
ATOM	338	CG	LEU 2	-	19.827	8.591	36.635	1.00 12.85	A
MOTA	339	CD1	LEU 3		21.007	9.367	36.066	1.00 16.06	A
MOTA	340	CD2	LEU A	4 40	20.293	7.526	37.650	1.00 17.91	A
ATOM	341	С	LEU A	40	16.763	10 046	38.497	1.00 10.71	A
ATOM	342	0	LEU A	40	16.848	10.258	39.701	1.00 11.30	A
ATOM	343	N	GLN 3	41	15.911	10.692	37.704	1.00 11.62	A

Figure 7H

ATOM	344	CA	GLN A	41	15 038	11.695	38.322	1.00 11.12	A
ATOM	345	CB	GLN A	41	14.241	12.447	37.257	1.00 11.92	A
MCTA	346	CG	GLN A	42	13.250	13.381	37.845	1.00 11.53	A
MOTA	347	CD	GLN A	41	12.230	13.933	36.838	1.00 12.64	A
ATOM	348	OE1	GLN A	41	11.814	13.226	35.962	1.00 13.16	A
ATOM	349	NE2	GLN A	41	11.972	15.220	36.973	1.00 13.67	A
ATOM	350	C	GLN A	41	14.081	11.031	39.332	1.00 10.98	A
ATOM	351	0	GLN A	41	13.883	11.585	40.404	1.00 12.39	A
ATOM	352	N	ALA A	4.2	13.571	9.845	38.994	1.00 12.53	A
ATOM	3 5 3	CA	ALA A	42	12.642	9.185	39.928	1.00 12.08	A
MOTA	354	CB	ALA A	4.3	12.035	7.954	39.295	1.00 13.83	A
ATOM	355	С	ALA A	42	13.383	8.856	41.218	1.00 14.57	A
ATOM	356	0	ALA A	42	12.820	8.975	42.296	1.00 15.73	A
MOTA	357	N	ARG A	43	14.647	8.446	41.147	1.00 13.64	A
MOTA	358	CA	ARG A	43	15.412	8.150	42.327	1.00 16,22	A
MOTA	359	CB	ARG A	. 43	16.772	7.626	41.852	1.00 18.06	A
MOTA	360	CG	ARG A	43	17.706	7.309	42.895	1.00 22.64	A
ATOM	361	CD	ARG A	43	17.232	6.108	43.679	1.00 25.20	A
MOTA	362	NE	ARG A	. 43	18.302	5.922	44.577	1.00 27.65	A
ATOM	363	CZ	ARG A	43	18.943	4.798	44.758	1.00 20.75	A
ATOM	364	NHl	ARG A	. 43	18.607	3.666	44.107	1.00 24.75	A
ATOM	365	NH2	ARG A	4.3	19.983	4.899	45.516	1.00 23.93	A
ATOM	366	С	ARG A	. 43	15.606	9.411	43.196	1.00 15.07	A
ATOM	367	^o	ARG A	. 43	15.441	9.372	44.435	1.00 17.46	A
MOTA	368	N	ILE A	44	15.930	10.529	42.553	1.00 14.44	A
ATOM	369	CA	ILE A	44	16.181	11.794	43.242	1.00 14.63	A
ATOM	370	CB	ILE A	44	16.801	12.854	42.280	1.00 15.70	A
ATOM	371	CG2	ILE A	44	16.817	14.226	42.941	1.00 16.89	A
ATOM	372	CGl	ILE A	44	18.236	12.422	41.940	1.00 16.08	A
ATOM	373	CD1	ILE A	44	18.765	13.127	40.739	1.00 19.48	A
ATOM	374	С	ILE A	44	14.906	12.326	43.887	1.00 16.35	A
ATOM	375	0	ILE A	44	14.984	12.862	44.991	1.00 19.28	A
ATOM	376	N	LEU A	45	13.747	12.150	43.258	1.00 15.72	A
ATOM	377	CA	LEU A	45	12.515	12.682	43.883	1.00 15.80	A
MOTA	378	CB	LEU A	45	11.505	13.032	42.801	1.00 15.66	A
ATOM	379	CG	LEU A	45	11.867	14.181	41.878	1.00 15.35	A
MOTA	380	CD1	LEU A	45	10.793	14.298	40.823	1.00 17.27	A
ATOM	381	CD2	LEU A	45	11.954	15.485	42.701	1.00 18.49	A
ATOM	382	С	LEU A	45	11.903	11.710	44.867	1.00 18.22	A
ATOM	383	0	LEU A	45	11.053	12.187	45.658	1.00 19.14	A
ATOM	384	TM	LEU A	45	12.258	10.488	44.884	1.00 20.39	A
MOTA	385	CA	ACE D	0	10.275	-0.794	28.942	1.00 41.14	В
ATOM	386	С	ACE D	0	11.674	-0.285	28.785	1.00 40.52	₿
ATOM	387	0	ACE D	D	11.905	0.677	28.016	1.00 41.12	В
ATOM	388	N	DLY D	1	12.631	-0.899	29.487	1.00 39.74	3
MOTA	389	CA	DLY D	1	13.997	-0.423	29.356	1.00 37.31	В
MOTA	390	C	DLY D	1	15.200	-1.051	30.044	1.00 35.38	B
ATOM	391	0	DLY D	1	15.133	-2.044	30.785	1.00 35.49	В
ATOM	392	N	DLA D	2	16.332	-0.424	29.752	1.00 33.19	В
ATOM	393	CA	DLA D	2	17.639	-0.797	30.279	1.00 31.99	В
ATOM	394	CB	DLA D	2	18.688	0.196	29.762	1.00 31.34	В
ATOM	395	С	DLA D	2	18.026	-2.217	29.871	1.00 31.71	3
ATOM	396	0	DLA D	2	18.611	-2.982	30.547	1.00 31.67	B
ATOM	397	N	DCS D	3	17.699	-2.577	28.640	1.0C 30.76	2
MOTA	398	CA	DCS D	3	18.061	-3.892	28.159	1.00 31.11	3
MOTA	399	С	DCS D	3	17.104	-4.987	28.618	1.00 31.69	3
MOTA	400	0	DCS D	3	17.531	-6.020	29.111	1.00 31.85	В
MOTA	401	CB	DCS D	3	18.128	-3.876	26.638	1.00 30.00	3

Figure 71

ATOM	402	SG	DCS	D	3	19.	502	-2.991	25.840	1.00	30.98	Ξ
ATOM	403	N	DLU		4	15.	813	-4.736	28.474	1.00	31.68	В
ATOM	404	CA	DLU		4	14.	782	-5.702	28.834		32.07	В
ATOM	405	CB	DLU		4		397	-5.090	28.574	1.00	33.43	В
ATOM	406	CG	DLU		4		060	-4.844	27.093		35.53	В
ATOM	407	CD	DLU		4	13.	663	-3.568	26.500		36.29	B
MOTA	408	OE1			4		422	~2.859	27.182		37.11	B
ATOM	409	OE2			4		367	-3.264	25.323	1.00		В
ATOM	410	C	DLU		4		875	-6.180	30.276		31,86	В
ATOM	411	Ō	DLU		4		832	-7.381	30.553		32.10	B
ATOM	412	N	DLA		5		022	-5.237	31.196		30.98	В
ATOM	413	CA	DLA		5		098	-5.566	32.611		30.61	В
ATOM	414	CB	DLA		5		984	-4.296	33.406	1.00	30.83	B
MOTA	415	C	DLA		5		362	-6.340	33.008		30.19	_ B
ATOM	416	ō	DLA		5		387	-7.044	34.027		30.60	В
ATOM	417	N	DRG		6		418	-6.202	32.216		29.09	B
MOTA	418	CA	DRG		6		673	-6.893	32.489	1.00	28.71	B
ATOM	419	CB	DRG		6		480	-8.408	32.369		31.46	B
ATOM	420	CG	DRG		6		169	-8.847	30.969		34.88	B
ATOM	421	CD	DRG		6		397	-8.762	30.070		37.42	В
MOTA	422	NE	DRG		6		715	-7.408	29.607		40.28	В
ATOM	423	CZ	DRG		6		121	-7.134	28.370		40.89	B
ATOM	424		DRG		6		248	-8.118	27.481		42.76	B
MOTA	425		DRG		6		409	-5.891	28.015		42.55	B
ATOM	426	C	DRG		6		313	-6.582	33.833		27.29	В
ATOM	427	Ô	DRG		6		994	-7.423	34.421		27.43	B
ATOM	428	N	DIS		7		100	-5.379	34.342		24.49	В
ATOM	429	CA	DIS		ż		731	-5.018	35,624		22.04	В
ATOM	430	CB	DIS		7		970	-3.888	36.284		22.68	B
ATOM	431	CG	DIS		7		555	-4.321	36.854		22.88	В
ATOM	432		DIS		; 7		178	-5.567	37.104		24.08	B
ATOM	433		DIS		7		650	-3.445	37.187		25.78	B
ATOM	434		DIS		7		595	-4.134	37.608		26,45	В
ATOM	435		DIS		7		894	-5.419	37.562		25.11	B
ATOM	435	C	DIS		7		156	-4.636	35.329		21.84	B
ATOM	437	0	DIS		7		412	-3.743	34.536		20.32	B
ATOM	438	N	DRG		8		091	-5.298	36.003		20.32	a B
ATOM	439	CA	DRG		8	23.		-5.122	35.778		19.80	В
ATOM	440	CB	DRG		8	24.		-5.994	36.755		20.87	13
ATOM	441	CG	DRG		8		175	-7.428	36.459		26.97	B
ATOM	442	CD	DRG		8	24.		-8.207	37.631		29.07	B
ATOM	443	NE	DRG		8	24.		-9.603	37.325		31.54	В
MOTA	444	CZ	DRG		8			-10.189	36.352		31.94	В
MOTA	445	NH1	DRG		8	26.		-9.485	35.658		33.88	В
ATOM	446	NH2	DRG		8		987		36.027		33.88	В
ATOM	447	C	DRG		8	23.		-3.711	35.873		17.95	B
ATOM	448	0	DRG		8	24.		-3.361	35.124		17.42	a B
ATOM	449	N	DLU		9	23.		-2.934	36.783		16.93	В
ATOM	450	CA	DLU		9	23.		-1.578	36.951		15.49	B
ATOM	451	CB	DLU		9	23.		-0.954	38.261		16.03	B
ATOM	452	CG	DLU		9	21.		-0.552	38.323		16.75	
		CD				20.		-1.816	38.786		16.82	B
MOTA	453 454		DLU		9	20. 21.		-2.982	38.584		19.63	В
ATOM ATOM	454 455		DLU		9 9	19.		-2.982 -1.498	39.310		20.12	B
ATOM	456	C	DLU		9	23.		-0.717	35.747		15.97	3 B
	457	0	DLU		. 9	24.		0.383	35.655		15.24	n 12
ATOM ATOM	457 458	Ŋ	DRP		10	22.		-1.186	34.844		15.66	B
ATOM	459	CA	DRP		10	22.		-0.435	33.611		15.31	В
WI OH		U.F.	للمالالبد	مد	± 0	. شه شم	* 0 2	- V - 200	JJ. 042	1.00		Ð

Figure 7J

ATOM	460	CE	DRP	ם	10	20 960	-0.18	7 33.420	1.00 16.05	В
ATOM	461	CG	DRP	, D	10	20.354	0.79	1 34.410	1.00 15.28	B
ATOM	462	CD2	DRP	D	10	20.504	2,200	34.384	1.00 15.28	£
MOTA	463	CE2	DRP	)	10	19.734	2.730	35.424	1.00 15.74	В
MOTA	464	CE3	DRP	D	10	21.237	3.075	33.563	1.00 15.47	Б
ATOM	465	CD1	DRP	D	10	19.504	0.513	35.449	1.00 16.40	В
ATOM	466	NE1	DRP	D	10	19.122	1.676		1.00 17.22	B
MOTA	457	CZ2			10	19.650			1.00 15.81	B
ATOM	468	CZ3			10	21.174			1.00 14.93	B
MOTA	469	CH2		D	10	20.382			1.00 15.26	В
ATOM	470	C	DRP		10	23.000			1.00 17.32	В
ATOM	471	ō	DRP		10	22.790			1.00 16.59	В
ATOM	472	N	DLA		11	23.744			1.00 17.72	В
MOTA	473	CA	DLA		11	24.253			1.00 18.88	B
ATOM	474	CB	DLA		11	25.034			1.00 20.11	B
ATOM	475	C	DLA		11	25.126			1.00 20.11	
ATOM	476	0	DLA		11	25.078				B
ATOM	477	N	DRP		12	25.884				В
ATOM	478	CA	DRP		12	26.759			1.00 17.86	В
		CB							1.00 17.72	B
ATOM	479		DRP		12	27.586			1.00 18.43	В
ATOM	480	CG	DRP		12	26.725	1.588		1.00 16.68	B
ATOM	481		DRP		12	26.285	2.900		1.00 16.49	B
MOTA	482		DRP		12	25.459	3.371		1.00 15.68	B
ATOM	483	CE3	DRP		12	26.519	3.714		1.00 17.14	B
ATOM	484				12	26.177	1.335		1.00 15.60	В
ATOM	485	NE1	DRP		12	25.402	2.400		1.00 15.74	В
ATOM	486	CZ2	DRP		12	24.842	4.628		1.00 15.78	В
MOTA	487	CZ3	DRP		12	25.904	4.977		1.00 17.42	B
ATOM	488		DRP		12	25.090	5.406		1.00 16.81	В
ATOM	489	C	DRP		12	25.913	0.577		1.00 18.81	В
ATOM	490	C	DRP		12	26.347	0.870		1.00 20.05	B
ATOM	491	N	DEU		13	24.740	1.020		1.00 17.43	В
ATOM	492	CA	DEU		1.3	23.915	1.866	28.926	1.00 17.59	₿
ATOM	493	CB	DEU		13	22.883	2.647	29.756	1.00 15.97	В
ATOM	494	CG	DEU		13	21.857	3.489	28.971	1.00 15.31	B
MOTA	495		DEU		13	22.559	4.585	28.204	1.00 15.99	3
ATOM	496		DEU		13	20.886	4.105	29.938	1.00 16.07	B
ATOM	497	C	DEU		13	23.265	1.011	27.847	1.00 19.32	В
ATOM	498	0	DEU		13	23.224	1.429	26.702	1.00 20.12	B
ATOM	499	N	DCS	D	14	22.775	-0.180	28.199	1.00 20.93	B
ATOM	500	CA	DCS		24	22.190	-1.046	27.196	1.00 22.79	В
ATOM	501	C	DCS		14	23.272	-1.329	26.124	1.00 22.54	В
ATOM	502	Q	DCS	D	14	22.963	-1.318	24.916	1.00 23.67	B
ATOM	503	CB	DCS	D	14	21.675	-2.319	27.874	1.00 23.47	B
MOTA	504	SG	DCS	D	14	21.216	-3.669	26.732	1.00 27.91	B
MOTA	505	N	DLA	D	15	24.514	-1.568	26.533	1.00 22.47	В
ATOM	506	CA	DLA	D	15	25.627	-1.857	25.614	1.00 23.31	3
MOTA	507	CB	DLA	D	15	26.868	-2.302	26.401	1.00 24.09	B
MOTA	508	C	DLA	D	15	25.987	-0.672	24.717	1.00 24.16	B
MOTA	509	0	DLA	D	15	26.511	-0.844	23.614	1.00 25.93	В
ATOM	510	N	DLA	D	16	25.723	0.544	25.192	1.00 22.60	В
ATOM	511	CA	DLA	D	16	26.017	1.743	24.400	1.00 22.10	B
ATOM	512	CB	DLA	D	16	26.006	2.985	25.314	1.00 22.02	В
ATOM	513	C	DLA	D	16	24.995	1.932	23.278	1.00 21.95	В
ATOM	514	0	DLA	D	16	25.355	2.570	22.256	1.00 32.36	В
ATOM	515	NT	DLA	D	16	23.843	1.460	23.410	1.00 03.47	В
MOTA	516	CL-1	CL	Ι	1	20.914	12.075	1.899	1.00 45.04	Ī
ATOM	517		WAT	W	1	23.911		-21.684	1.00 53.50	W

Figure 7K

MOTA	518	OH2 WAT W	2	30.822	2.444	-19.357	1.00 52.17	W
MOTA	519	OHO WAT W	3	30.369	13.971	-17.693	1.00 37.33	W
ATOM	520	W TAW CHO	4	27.699	12.875	-16.588	1.00 46.63	W
MOTA	521	OH2 WAT W	5	23.417	1.727	-13.168	1.00 48.41	W
MOTA	522	OHI WAT W	б	24.012	1.401	-16.007	1.00 58.65	W
MOTA	523	OHI WAT W	7	16.572	3.069	-7.418	1.00 36.12	W
ATOM	524	OH2 WAT W	8	32.381	11.028	-8.334	1.00 55.01	W
ATOM	525	OH2 WAT W	9	33.753	7.275	-10.261	1.00 53.14	W
ATOM	526	OHO WAT W	10	20.318	-0.862	-12.067	1.00 28.89	W
ATOM	527	OH2 WAT W	11	26.434	1.459	-10.129	1.00 43.04	W
ATOM	528	OH2 WAT W	12	27.878	0.323	-12.146	1.00 55.95	W
ATOM	529	OH2 WAT W	13	31.427	0.259	-10.741	1.00 52.47	W
ATOM	530	OH2 WAT W	14	29,889	8.411	-6.889	1.00 56.49	W
ATOM	531	OH2 WAT W	15	22.532	1.843	-4.021	1.00 32.19	W
ATOM	532	OH2 WAT W	16	23.814	-0.534	-4.336	1.00 39.56	w
ATOM	533	OH2 WAT W	17	19.996	1.598	-5.292	1.00 33.28	W
ATOM	534	OH2 WAT W	18	25.262	-3.040	-8.386	1.00 28.37	W
ATOM	535	OH2 WAT W	19	22,556	0.000	0.001	1.00 30.95	W
ATOM	536	OH2 WAT W	20	24.369	-1.421	-1.823	1.00 29.32	W
ATOM	537	OH2 WAT W	21	29.134	-0.583	-6.291	1.00 46.18	W
ATOM	538	OHO WAT W	22	27.394	2,286	-5.533	1.00 43.67	W
ATOM	539	OH2 WAT W	23	26.774	0.049	-4.387	1.00 45.47	w
MOTA	540	OH2 WAT W	24	30.008	5.236	1.507	1.00 52.80	W
MOTA	541	OH2 WAT W	25	27.776	4.560	0.356	1.00 42.94	M
MOTA	542	OH2 WAT W	26	32.018	6.237	0.261	1.00 53.15	W
ATOM	543	OH2 WAT W	28	18.650	4.426	-0.423	1.00 34.71	W
ATCM	544	OH2 WAT W	29	18.919	1.842	-1.284	1.00 42.23	M
ATOM	545	OHE WAT W	30	11.826	6.239	7.700	1.00 59.49	M
MOTA	546	OH2 WAT W	31	13.683	5.469	2.919	1.00 52.76	W
ATOM	547	OH2 WAT W	32	16.956	4.594	1.380	1.00 47.84	W
ATOM	548	OH2 WAT W	33	17.260	2.099	7.679	1.00 46.32	W
ATOM	549	OH2 WAT W	34	17.636	1.737	-4.073	1.00 51.94	W
ATOM	550	OH2 WAT W	35	16.221	5.835	9.764	1.00 30.19	W
ATOM	551	OH2 WAT W	36	26.030	8.926	8.979	1.00 51.32	W
ATOM	552	OH2 WAT W	37	13.758	2.898	9.624	1.00 51.32	W
ATOM	553	OH2 WAT W	38	14.899	5.914	11.925	1.00 35.86	W
ATOM	554	OH2 WAT W	39	19.841	0.030	14.724	1.00 45.90	W
ATOM	555	OH2 WAT W	40	13.772	2.335	12.179	1.00 50.60	W
ATOM	556	OH2 WAT W	41	13.367	0.805	6.229	1.00 51.80	W
ATOM	557	OH2 WAT W	42	15.587	3.501	15.845	1.00 30.05	W
ATOM	558	OH2 WAT W	43	14.280	4.098	13.819	1.00 48.74	W
ATOM	559	OH2 WAT W	44	14.273	3.983	18.042	1.00 32.52	W
ATOM	560	OH2 WAT W	45	14.275	2.720	20.720	1.00 40.19	W
ATOM	561	OH2 WAT W	46	21.969	2.228	18.885	1.00 22.32	W
ATOM	562	OH2 WAT W	47	21.588	1.778	21.594	1 00 28.43	M
ATOM	563	OH2 WAT W	48	11.908	3.300	22.023	1.00 50.50	W
ATOM	564	OH2 WAT W	49	13.679	0.626	18.643	1.00 46.64	W
MOTA	565	OH2 WAT W	50	16.369	2.196	22.597	1.00 30.08	W
ATOM	566	OH2 WAT W	51	12.828	6.527	18.634	1.00 30.08	W
ATOM	567	OH2 WAT W	52	24.603	2.631	19.581	1.00 37.29	
ATOM	568	OH2 WAT W	53	11.867	0.791	23.131	1.00 23.33	W
ATOM	569	OH2 WAT W	54	24.546	5.366	17.812	1.00 50.24	
ATOM	570	OH2 WAT W	55	20.954	0.091	17.131	1.00 49.14	W
		OH2 WAT W	55 56	19.747	-0.562	21.394	1.00 49.14	W
ATOM	571 572							W
ATOM	572	OH2 WAT W	57	14.819	8.442	19.922	1.00 33.61	W
ATOM	573 574		58	10.854	5.349	19.724	1.00 45.89	W
ATOM	574	OH2 WAT W	59	10.710	9.378	19.376	1.00 37.52	W
ATOM	575	OH2 WAT W	60	10.497	10.303	21.845	1.00 34.96	W

Figure 7L

ATOM	576	OH2 WAT W 61	12.866	5.691	26.354	1 00 28.86	W
$A$ $^{m}O$ $^{m}$	577	OH2 WAT W 62	10.758	7.878	25.495	1.00 42.32	W
MOTA	578	OH2 WAT W 63	11.782	6.555	28.773	1.00 29.65	W
ATOM	579	OH2 WAT W 64	10.296	8.472	27.988	1.00 37.31	W
ATOM	580	OHO WAT W 65	13.316	2.342	26.849	1.00 43.22	W
ATOM	581	OHI WAT W 66	29.863	-1.693	28.654	1.00 38.41	W
ATOM	582	OH2 WAT W 67	16.468	-1.186	26.444	1.00 32.71	M
ATOM	583	OH2 WAT W 68	20.934	12.065	25.212	1.00 18.68	W
ATOM	584	OH2 WAT W 69	7.101	5.989	26.485	1.00 48.02	W
ATOM	585	OH2 WAT W 70	7.226	10.744	27.574	1.00 33.30	W
MOTA	586	OH2 WAT W 71	16.382	-1.374	34.997	1.00 34.36	W
ATOM	587	OH2 WAT W 72	17.474	-0.717	38.167	1.00 28.82	W
ATOM	588	OH2 WAT W 73	17.984	-2.951	33.186	1.00 27.39	W
ATOM	589	OH2 WAT W 74	16.999	1.929	37.830	1.00 37.09	W
ATOM	590	OH2 WAT W 75	20.595	3.071	39.121	1.00 19.51	W
MOTA	591	OH2 WAT W 76	14.326	5.004	39.584	1.00 20.31	W
ATOM	592	OH2 WAT W 77	11.973	4.544	38.034	1.00 32.93	W
ATOM	593	OH2 WAT W 78	18.317	4.417	39.397	1.00 44.00	W
MOTA	594	OH2 WAT W 79	10.983	-2.804	30.948	1.00 52.39	W
ATOM	595	OH2 WAT W 80	11.064	0.945	32.640	1.00 30.78	W
ATOM	596	OH2 WAT W 81	12.861	0.902	39.566	1.00 51.74	W
ATOM	597	OH2 WAT W 82	14.353	-1.379	39.210	1.00 48.06	W
ATOM	598	OH2 WAT W 83	13.014	-3.417	36.263	1.00 46.54	W
ATOM	599	OH2 WAT W 84	11.101	-2.319	39.669	1.00 61.24	W
ATOM	600	OH2 WAT W 85	20.879	-3.825	31.838	1.00 26.25	W
MOTA	501	OH2 WAT W 86	24.470	-4.753	28.192	1.00 36.86	W
ATOM	602	OH2 WAT W 87	22.117	-5.700	29.831	1.00 38.03	W
ATOM	603	OH2 WAT W 88	19.685	0.721	41.041	1.00 28.21	W
ATOM	604	OH2 WAT W 89	20.274	5.127	40.337	1.00 32.29	W
ATOM	605	042 WAT W 90	10.072	4.538	29.943	1.00 33 10	W
ATOM	606	OH2 WAT W 91	10.573	4.216	33.496	1.00 33.22	M
ATOM	607	OHI WAT W 92	10.336	5.922	36.364	1.00 48.48	W
MOTA	608	OH2 WAT W 93	9.113	5.209	40.332	1.00 51.71	W
ATOM	609	OH2 WAT W 94	9.980	8.713	42.573	1.00 24.98	W
ATOM	610	OH2 WAT W 95	17.708	6.542	-1.798	1.00 36.93	W
MOTA	611	OH2 WAT W 96	10.278	11.397	38.730	1.00 17.13	W
MOTA	612	OH2 WAT W 97	11.290	10.478	36.184	1.00 15.62	W
ATOM	613	OH2 WAT W 98	8.444	12.988	37.395	1.00 17.25	W
ATOM	514	OH2 WAT W 99	8.735	9.911	40.361	1.00 25.18	W
ATOM	615	OH2 WAT W 100	6.665	11.917	35.865	1.00 28.95	W
MOTA	616	OH2 WAT W 101	8.907	9.736	35.113	1.00 28.77	M
ATOM	617	OH2 WAT W 102	10.416	5.919	42.300	1.00 32.80	W
ATOM	618	OH2 WAT W 103	8.278	3.600	38.536	1.00 54.85	W
ATOM	619	OHO WAT W 104	14.183	7.249	45.734	1.00 23.53	M
ATOM	620	CH2 WAT W 105	11.426	7.965	46.547	1.00 34.68	W
MOTA	621	OH2 WAT W 106	16.907	2.218	41.970	1.00 39.50	W
ATOM	622	OH2 WAT W 107	16.479	14.336	46.761	1.00 23.72	M
ATOM	623	OH2 WAT W 108	8.319	12.931	45.022	1.00 22.11	W
ATOM	624	OHI WAT W 109	7.189	12.423	42.385	1.00 39.34	W
MOTA	625	OH1 W TAW 110	8.599	9.769	44.603	1.00 40.15	M
ATOM	626	OH2 WAT W 111	26.891	-1.858	33.829	1.00 23.69	W
ATOM	627	OH2 WAT W 112	28.775	-3.310	32.521	1.00 38.13	W
MOTA	628	OH2 WAT W 113	31.335	0.587	33.068	1.00 34.37	W
MOTA	629	OH2 WAT W 114	30.921	-0.919	36.513	1.00 44.24	W
ATOM	630	OH2 WAT W 115	30.098	2.733	29.619	1.00 39.50	W
MOTA	631	OH2 WAT W 116	33.465	2.665	34.521	1.00 52.27	W
MOTA	632	OH2 WAT W 117	25.612	14.159	-18.301	1.00 56.10	W
ATOM	633	OH2 WAT W 118	33.904	2.165	-15.960	1.00 57.70	W

Figure 7M

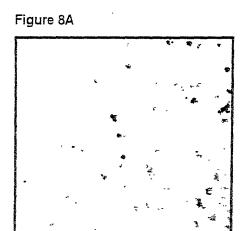
END

Docket/App No.: 0399.1192-008
Title: Inhibitors of HIV Membrane Fusion

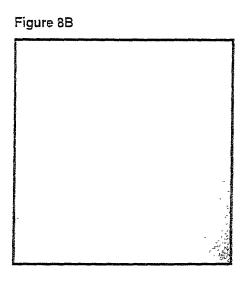
Debra M. Eckert, et al. Inventors:

MOTA	634	OH2	WAT	W	119	33.766	4 21 5	-14.106	1 00	57.44	7.4
ATOM	635	OH2	WAT			26.831		7.075		40.38	W
MOTA	636	OH2	WAT		121	26.562		4.240			W
ATOM	637	OH2	WAT	W	122	29.081	7.039	-		32.00	W
ATOM					123			3.251		46.30	W
	638	OH2	WAT			22.080		10.516		39.31	W
ATOM	639	OH2	WAT			28.185		13.044		45.28	W
MOTA	640	OH2	WAT	W	125	29.400	7.324	10.996		52.21	W
ATOM	641	OH2	WAT		126	12.966	3.595	24.673		59.42	W
ATOM	642	OH2	WAT	W	127	8.932	7.961	36.476		45.85	W
ATOM	643	OH2	WAT	W	128	12.712	5.206	41.719	1.00	38.55	W
ATOM	644	OH2	WAT	M	129	9.431	10.564	47.230	1.00	35.27	W
ATOM	645	OH2	WAT	W	130	6.643	9.576	45.596	1.00	44.00	W
ATOM	646	OH2	TAW	W	131	21.501	13.657	45.856	1.00	43.49	W
ATOM	647	OH2	WAT	W	132	19.368	14.112	46.567	1.00	41.15	W
ATOM	648	OH2	WAT	W	133	20.913	12.058	48.230	1.00	36.86	W
ATOM	649	OH2	WAT	W	134	13.556	4.967	44.137	1.00	49.55	W
ATOM	650	OH2	WAT	W	135	17.568	0.000	0.010	1.00	54.94	W
ATOM	651	OH2	TAW	W	136	17.847	-0.139	11.093	1.00	42.03	W
ATOM	652	OH2	WAT	W	137	25.734	4.074	15.641	1.00	35.36	W
ATOM	653	OH2	WAT	W	138	8.107	7.930	38.831	1.00	37.47	W
ATOM	654	OH2	WAT	W	139	10.614	4.603	44.378	1.00	61.10	W
MOTA	655	OH2	WAT	W	140	14.180	-9.552	32.610	1.00	37.66	W
MOTA	656	OH2	WAT	W	141	26.549	-4.072	22.858	1.00	48.05	W
MOTA	657	OH2	TAW	W	142	21.688	-2.141	22.847	1.00	36.75	W
ATOM	658	OH2	WAT	W	143	15.457	1.462	27.799	1.00	38.11	W
MOTA	659	OH2	WAT	W	144	18.956	16.356	45.521	1.00	36.93	W
ATOM	660	OH2	WAT	W	145	15.655	2.938	40.183	1.00	40.77	W
MOTA	661	OH2	WAT	W	146	15.688	-1.613	19.777	1.00	17.04	W
MOTA	662	OH2	WAT	W	147	26.880	-5.627	28.327	1.00 4	44.89	W
MOTA	663	OH2	WAT	W	148	28.682	-5.605	33.707	1.00 4	13.34	W
ATOM	664	OH2	WAT	W	149	28.220	11.179	-23.836	1.00	53.67	W
MOTA	665	OH2	WAT	W	150	27.905	3.222	-7.774	1.00 4	14.54	W
ATOM	666	OH2	WAT	W	151	15.403	-11.541	32.995	1.00 4	17.59	W
TER											

### Inhibition of HIV-1 Membrane Fusion by a D-Peptide



Syncytia Assay with no D-peptide



Syncytia Assay with [100 µM] peptide

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

Inventors:

Debra M. Eckert, et al.

## NMR Characterization of Aromatic Residues in **IQN17/D-Peptide Complexes**

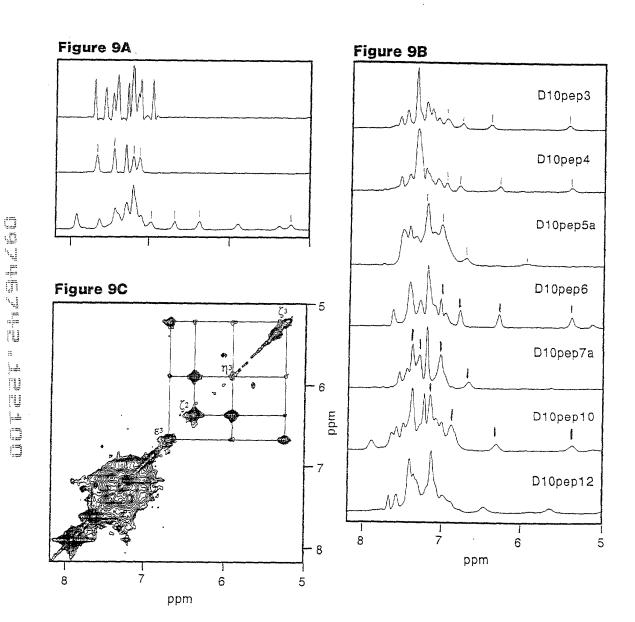
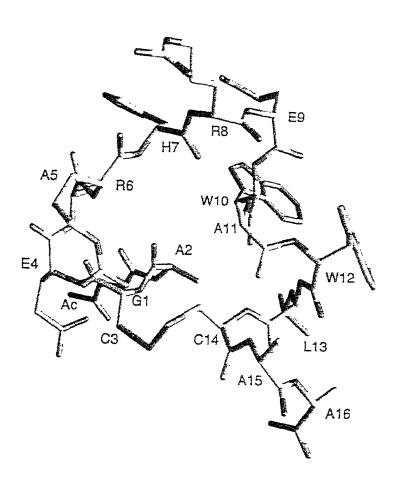


Figure 10: Conformation of D10pep1 in complex with IQN17



CRYST1	57.	935	121	. 953	73.6	69 90.0	00.00	90.00	C2221	1
ORIGX1		1.00	0000	0.	.000000	0.00000	0	0.00000		
ORIGX2		0.00	0000	1.	000000	0.00000	0	0.00000		
ORIGX3			0000		000000	1.00000		0.00000		
SCALE1			7261		000000	0.00000		0.00000		
					.008199					
SCALE2			0000			0.00000		0.00000		
SCALE3			0000		000000	0.01357		0.00000		
ATOM	1	CA	ACE	A	0	25.795	17.140	37.286	1.00 61.	.88 A
ATOM	2	С	ACE	Ą	0	25.799	18.376	36.435	1.00 62.	.00 A
ATOM	3	0	ACE	A	0	25,500	19.475	36.921	1.00 62.	10 A
ATOM	4	N	ARG		1	26.134	18.217	35.157	1.00 60.	
ATOM	5	CA	ARG		1	26,203	19.328	34.217	1.00 60.	
ATOM	6	CB	ARG		1	27.212	18.993	33.110	1.00 61.	
ATOM	7	CG	ARG		1	27.630	20.135	32.212	1.00 60.	
MOTA	8	CD	ARG		1	28.500	19.587	31.097	1.00 64.	
ATOM	9	NE	ARG	A	1	29.018	20,628	30.217	1.00 65.	07 A
ATOM	10	CZ	ARG	A	1.	29.706	20.377	29.109	1.00 63.	90 A
ATOM	11	NH1	ARG	A	1	29.951	19.124	28.766	1.00 64.	20 A
ATOM	12	NH2	ARG	A	1	30.157	21.367	28.351	1.00 63.	51 A
ATOM	13	С	ARG		1	24.823	19.573	33.595	1.00 59.	
ATOM	14	Õ	ARG		1	24.453	20.714	33.294	1.00 57.	
	15		MET			24.065		33.425	1.00 57.	
ATOM		N		A	2 .		18.494			
ATOM	16	CA	MET		2	22.736	18.573	32.836	1.00 59.	
ATOM	17	CB	MET	Α	2	22.273	17.198	32.397	1.00 59.	
ATOM	18	CG	MET	A	2	21.204	17.251	31.342	1.00 63.	56 A
ATOM	19	SD	TMM	A	2	20.044	15.905	31.454	1.00 67.	77 A
ATOM	20	CE	MET	A	2	19.089	16.438	32.857	1.00 66.	61 A
ATOM	21	C	MET	A	2	21.723	19.130	33.834	1.00 61.	33 A
ATOM	22	0		A	2	20.543	19.276	33.521	1.00 59.	
ATOM	23	N	LYS		3	22.200	19.417	35.041	1.00 62.	
ATOM	24	CA	LYS		3	21.373	19.961	36.107	1.00 63.	
ATOM	25	CB	LYS		3	21.817	19.361	37.449	1.00 64.	
ATOM	26	CG	LYS		3	20.982	19.721	38.687	1.00 54.	
ATOM	27	CD	LYS		3	21.195	21.159	39.160	1.00 64.	-
ATOM	28	CE	LYS		3	20.543	21.405	40.525	1.00 64.	
ATOM	29	NZ	LYS	A	3	19.077	21.123	40.548	1.00 63.	04 A
ATOM	30	С	LYS	A	3	21.599	21.467	36.062	1.00 64.	55 A
ATOM	31	0	LYS	A	3	20.639	22.245	36.032	1.00 64.	65 A
ATOM	32	N	GLN	Α	4	22.869	21.873	36.036	1.00 64.	34 A
ATOM	33	CA	GLN		4	23.232	23.289	35.952	1.00 65.	
ATOM	34	СВ	GLN		4	24.746	23.447	35.780	1.00 67.	
ATOM	35	CG	GLN		4	25.552	22.954	36.963	1.00 71.	
ATOM	36	CD	GLN		4	25.297	23.771	38.212	1.00 75.	
ATOM	37	OE1	GLN		4	25.618	24.962	38.269	1.00 77.	
ATOM	38	NE2	GLN		4	24.706	23.135	39.225	1.00 76.	
MOTA	39	С	GLN		4	22.508	23.928	34.758	1.00 64.	
ATOM	40	0	GLN	A	4	22.191	25.128	34.776	1.00 62.	A 80
ATOM	41	N	ILE		5	22.260	23.120	33.726	1.00 59.	
MOTA	42	CA	ILE	A	5	21.540	23.587	32.552	1.00 58.	22 A
ATOM	43	CB	ILE	A	5	21.567	22.558	31.398	1.00 56.	85 A
ATOM	44	CG2	ILE	A	5	20.438	22.851	30.416	1.00 53.	
ATOM	45		ILE		5	22.942	22.562	30.719	1.00 56.	
ATOM	46	CD1			5	23.079	21.524	29.514	1.00 59.	
						20.083				
ATOM	47	C	ILE		5		23.828	321.929	1.00 58.	
ATOM	48	0	ILE		5	19.575	24.928	32.729	1.00 58.	
ATCM	19	N	GLU		6	19.424	22.796	33.472	1.00 59.	
ATOM	50	CA	GLJ		6	18.013	22.883	33.377	1.00 56.	
ATCM	51	CB	GLU	$\mathcal{A}$	ő	17.528	21.537	34.448	1.00 55,	59 A

Figure 11A

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM CG GLU A 17.638 20.359 33.480 1.00 56.46 CD GLU A 17.293 19.009 34.119 ATOM 53 1.00 56.33 6 ATOM 54 OE1 GLU A б 17.702 18.790 35.278 1.00 53,43 ATOM 55 OE2 GLU A б 16.644 18.157 33 458 1.00 55.03 GLU A 17.873 23.977 34.926 ATOM 56 С 1.00 54.87 6 16.793 ATOM 57 0 GLU A 6 24.509 35.137 1.00 52.82 MOTA N ASP A 18.986 24.300 35.572 1.00 55.62 7 19.039 25.336 36.597 ATTOM 59 CA ASP A 1.00 56.65 37.451 25.162 CB 20,291 ATOM 60 ASP A 1.00 57.46 ATOM 61 CG ASP A 7 20.010 24.471 38.762 1.00 57.37 ATOM 62 OD1 ASP A 19.180 23.534 38.775 1.00 53.78 7 OD2 ASP A 20.637 24.862 39.771 ATOM 63 1.00 57.66 ATOM 64 С ASP A 7 19.034 26.745 36.041 1.00 56.99 65 ASP A 18.516 27.662 36.678 ATOM 0 1.00 55.43 8 19.532 26.945 34.873 MOTA 66 N LYS A 1.00 58.30 MOTA 67 CA LYS A 8 19.642 28.290 34.312 1.00 59.87 MOTA 68 CB LYS A 8 20.971 28.599 33.612 1.00 62 61 34.487 22.203 28.372 CG LYS A 1.00 66.85 ATOM 69 8 ATOM 70 CD LYS A 8 23.232 29.498 34.357 1.00 70.21 30.576 35.293 ATOM 71 CE LYS A 8 22.915 1.00 72.00 72 NZ LYS A 21.583 31.323 35.091 1.00 72.05 ATOM 8 ATOM 73 C LYS A 8 18,467 28.481 33.354 1.00 58.08 74 0 LYS A 8 18.145 29.609 32.969 ATOM 1.00 56.44 Α 9 17.835 27.376 32.967 1.00 55.29 75 ILE A MOTA N ð 6 MOTA 76 CA ILE A 16.668 27.436 32.099 1.00 56.69 MOTA 77 CB ILE A 16.325 26.052 31.486 1.00 54.89 78 CG2 ILE A 9 14.892 26.067 30.915 1.00 54.20 ATOM CG1 ILE A 9 CD1 ILE A 9 17.373 79 25.676 30.423 1.00 55.96 MOTA ATOM 80 17.131 24.339 29.717 1.00 54.22 15.526 27.876 ATOM 81 C ILE A 9 33.018 1.00 57.98 9 14.603 28.572 32.616 1.00 55.85 ATOM 82 0 ILE A GLU A 10 27.458 ATOM 83 N 15.626 34.271 1.00 59.96 ATOM 84 CA GLU A 10 14.641 27.788 35.283 1.00 61.12 ATOM 85 CB GLU A 10 14.850 26.901 36.510 1.00 63.01 CG GLU A 10 13.846 27.117 37.618 1.00 66.89 ATOM 86 Ā MOTA 87 CD GLU A 10 14.387 26.672 38.955 1.00 68.37 MOTA 88 OE1 GLU A 10 14.844 25.510 39.054 1.00 67.70 OE2 GLU A 10 14.355 27.487 39.903 1.00 68.42 MOTA 89 ATOM 90 C GLU A 10 14.872 29.243 35.664 1.00 59.41 91 GLU A 10 13.947 29.958 36.037 1.00 59.95 ATOM 0 16.127 ATOM 92 N GLU A 11 29.663 35.565 1.00 57.16 CA GLU A 11 93 31.024 ATOM 16.524 35.893 1.00 55.88 ATOM 94 CB GLU A 11 18.042 31.095 36.019 1.00 58.17 36.527 ATOM 95 CG GLU A 11 18.569 32.375 1.00 62,73 GLU A 11 18.459 32.382 38.139 1.00 67.75 ATOM 96  $^{\rm CD}$ Α Q7 31.512 38.782 ATOM OE1 GLU A 11 19.101 1.00 67.91 ATOM 98 OE2 GLU A 11 17.736 33.249 38.681 1.00 68.84 MOTA 99 GLU A 11 16.056 31.976 34.789 1.00 54.76 С Д GLU A 11 15.805 33.160 35.030 1.00 54.78 ATOM 100 0 MOTA 101 ILE A 12 15.945 31 443 33.575 1.00 52.61 MOTA 102 CA ILE A 12 15.510 32.210 32.414 1,00 50.09 Α ILE A 12 CB 16.002 31.096 1.00 50.23 31.548 ATOM 103 A ATOM 104 CG2 ILE A 12 15.201 32.073 29.905 1.00 48.54 17.508 31.773 30.930 1.00 50.30 ATOM 105 CG1 ILE A 12 А 106 CD1 ILE A 12 18.114 31.062 29.724 ATOM 1.00 53.10 32.362 1.00 49.83 32.017 1.00 47.70 MOTA 107 ILE A 12 13.988 32.324 108 12 13.447 33.376 MOTA ILE A MCTA 109 GLU A 13 13.306 31.232 32.698 1.00 48.57

Figure 11B

31.218

29.810

11.849

11.320

32.677

1.00 48.22

32.954 1.00 45.44

CA GLU A 13 CB GLU A 13

ATOM

ATOM

110

111

ATOM	112	CG	GLU	A	13	11.673	28.794	31.895	1.00 46.65	A
ATOM	113	CD	GLU		13	11.419	27.372	32.358	1.00 49.90	Ā
ATOM	114	OE1			13	12.051	26.968	33.366	1.00 49.96	A
ATOM	115	OE3	GLU		13	10.599	26.665	31.720	1.00 50.18	A
ATOM	116	C	GLU		13	11.357	32.163	33.749	1.00 47.83	A
MOTA	117	0	GLU		13	10.279	32.731	33.638	1.00 48.72	A
ATOM	118	N	SER	A	14	12.168	32.313	34.786	1.00 48.67	A
ATOM	119	CA	SER		14	11.862	33.187	35.907	1.00 49.89	A
ATOM	120	CB	SER		14	12.906	32.985	37.014	1.00 49.05	A
ATOM	121	OG	SER	Α	14	12.634	33.773	38.160	1.00 49.35	A
ATOM	122	С	SER	A	14	11.885	34.527	35.415	1.00 50.52	A
ATOM	123	0	SER		14	10.869	35.313	35.431	1.00 54.15	A
ATOM	124	N	LYS	A	15	13.056	35.067	34.971	1.00 49.27	A
ATOM	125	CA	LYS		15	13.248	36.416	34.474	1.00 51.02	A
ATOM	126	CB	LYS		15	14.707	36.589	34.042	1.00 54.30	A
ATOM	127	CG	LYS	Α	15	15.018	37.931	33.417	1.00 58.79	A
ATOM	128	CD	LYS		15	14.843	39.039	34.437	1.00 63.42	A
ATOM	129	CE	LYS	A	15	15.841	38.880	35.576	1.00 65.66	A
ATOM	130	NZ	LYS	A	15	15.722	39.983	36.569	1.00 68.14	A
ATOM	131	C	LYS	A	15	12.313	36.758	33.305	1.00 50.99	A
ATOM	132	0	LYS	A	15	12.022	37.926	33.061	1.00 49.62	A
ATOM	133	N	GLN	A	16	11.848	35.740	32.587	1.00 50.06	A
MOTA	134	CA	GLN	Α	16	10.965	35.937	31.444	1.00 49.96	A
ATOM	135	CB	GLN	A	16	10.950	34.584	30.570	1.00 49.89	A
ATOM	136	CG	GLN	A	16	10.133	34.810	29.286	1.00 50.59	A
ATOM	137	CD	GLN	A	16	10.287	33.603	28.369	1.00 54.27	A
MOTA	138	OE1	${\tt GLN}$	Α	16	9.799	32.511	28.667	1.00 56.28	A
ATOM	139	NE2	GLN	A	16	10.985	33.796	27.250	1.00 54.69	A
ATOM	140	C	GLN	A	16	9.551	36.256	31.899	1.00 50.61	A
MOTA	141	0	GLN	A	16	8.788	36.931	31.195	1.00 48.56	A
ATOM	142	N	LYS	A	17	9.198	35.736	33.067	1.00 49.38	A
ATOM	143	CA	LYS		17	7.883	35.973	33.623	1.00 49.73	A
MOTA	144	CB	LYS		17	7.582	34.982	34.750	1.00 52.97	A
ATOM	145	CG	LYS		17	6.250	35.226	35.448	1.00 56.86	A
ATOM	146	CD	LYS		17	6.066	34.276	36.618	1.00 59.31	A
ATOM	147	CE	LYS		17	4.763	34.552	37.354	1.00 59.95	A
ATOM	148	NZ	LYS		17	4.592	33.621	38.506	1.00 62.05	A
ATOM	149	С	LYS		17	7.927	37.390	34.163	1.00 48.25	A
ATOM	150	0	LYS		17	6.977	38.144	34.008	1.00 47.73	A
ATOM	151	N	LYS		18	9.043	37.750	34.791	1.00 45.58	A
ATOM	152	CA	LYS		18	9.190	39 101	35.309	1.00 45.26	A
ATOM	153 154	CB	LYS		18	10.523	39.270	36.047	1.00 47.34	A
ATOM ATOM	155	CD	LYS		18 18	10.627 11.831	38.493 38.976	37.362 38.168	1.00 50.10	A
ATOM	156	CE	LYS		18	11.851	38.358	39.550	1.00 52.93 1.00 55.07	A
ATOM	157	NZ	LYS		18	12.933	38.968	40.398	1.00 59.20	A
ATOM	158	C	LYS		18	9.107	40.110	34.171	1.00 33.20	A A
ATOM	159	0	LYS		18	8.585	41.206	34.349	1.00 42.70	A
ATOM	160	N	ILE		19	9.633	39.740	33.008	1.00 40.25	A
ATOM	161	CA	ILE		19		40.595	31.831	1.00 39.53	A
ATOM	162	CB	ILE		19	10.494	40.015	30.710	1.00 42.08	A
ATOM	163		ILE		19	10.133	40.631	29.369	1.00 41.71	A
ATOM	164		ILE		19	11.969	40.214	31.074	1.00 42.52	A
ATOM	165		ILE		19	12.939	39.656	30.039	1.00 43.29	A
ATOM	166	C	ILE		19	8.172	40.725	31.325	1.00 39.27	Ā
ATOM	167	0	ILE		19	7.751	41.790	30.899	1.00 37.81	A
MOTA	168	N	GLU		20	7.421	39.637	31.372	1.00 39.00	A
ATOM	169	CA	GLU		20	6.036	39.692	30.930	1.00 40.27	A
MOTA	170	CB	GLU		20	5.437	38.280	30.834	1.00 43.21	A
MOTA	171	CG	GLU		20	5.898	37.474	29.606	1.00 48.10	A

Figure 11C

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM	172	CD	GLU	A	20	5.446	36.019	29.659	1.00 50.57	A
ATOM	173	OEl	GLU	Α	20	5.832	35.316	30.617	1.00 52.42	A
ATOM	174	OE3	GLU	A	20	4.708	35.575	28.752	1.00 52.16	A
MCTA	175	С	GLU	A	20	5.195	40.546	31.873	1.00 46.09	A
MOTA	176	0	GLU	A	20	4.148	41.056	31.480	1.00 40.96	A
MOTA	177	N	ASN		21	5.637	40.694	33.119	1.00 38.83	A
ATOM	178	CA	ASN	À	21	4.880	41.498	34.071	1.00 40.69	A
ATOM	179	CB	ASN	A	21	5.216	41.107	35.507	1.00 39.42	A
ATOM	180	CG	ASN		21	4.618	39.768	35.892	1.00 41.35	A
ATOM	181	OD1	ASN		21	3.905	39.151	35.102	1.00 38.98	A
ATOM	182	ND2			21	4.902	39.312	37.107	1.00 40.82	A
MOTA	183	C	ASN		21	5.163	42.958	33.846	1.00 42.25	A
ATOM	184	0	ASN		21	4.261	43.801	33.872	1.00 42.61	A
ATOM	185	N	GLU		22	6.432	43.244	33.602	1.00 41.94	A
ATOM	186	CA	GLU		22	6.893	44.589	33.343	1.00 41.44	A
MOTA	187	CB	GLU		22	8.403	44.563	33.127	1.00 43.01	A
MOTA	188	CG	GLU		22	9.126	45.861	33.421	1.00 49.75	A
ATOM	189	CD	GLU		22	9.769	45.872	34.802	1.00 52.80	A
ATOM	190	OE1			22	10.611	44.988	35.077	1.00 53.66	A.
ATOM	191	OE2	GLU		22	9.447	46.764	35.608	1.00 57.41	A
ATOM	192	C	GLU		22	6.188	45.082	32.068	1.00 41.34	A
ATOM	193	0	GLU		22	5.851	46.263	31.954	1.00 43.52	A
ATOM	194	N	ILE		23	5.964	44.175	31.116	1.00 37.55	A
ATOM	195	CA	ILE		23	5.295	44.530	29.863	1.00 35.10	A
ATOM ATOM	196 197	CB CG2	ILE		23	5.418	43.408	28.800	1.00 36.19	A
ATOM	198	CG1	ILE		23 23	4.520	43.719	27.592	1.00 35.94	A
ATOM	199	CD1	ILE		23	6.876 7.122	43.288	28.340	1.00 39.18	A
ATOM	200	C	ILE		23	3.816	44.827	27.324	1.00 40.80 1.00 33.36	A
ATOM	201	0	ILE		23	3.284	45.796	29.568	1.00 28.55	A
ATOM	202	Ŋ	ALA		24	3.167	43.798	30.881	1.00 22.55	A
ATOM	203	CA	ALA		24	1.750	44.147	31.179	1.00 30.41	A.
ATOM	204	CB	ALA		24	1.276	42.994	32.043	1.00 27.29	A A
ATOM	205	C	ALA		24	1.531	45.479	31.893	1.00 27.29	A
ATOM	206	0	ALA		24	0.562	46.183	31.608	1.00 31.49	Ā
ATOM	207	N	ARG		25	2.428	45.825	32.816	1.00 30.94	A
ATOM	208	CA	ARG		25	2.297	47.070	33.547	1.00 30.44	A
ATOM	209	CB	ARG		25	3.197	47.066	34.798	1.00 32.01	A
ATOM	210	ÇG	ARG		25	2.727	46.101	35.894	1.00 34.49	A
ATOM	211	CD	ARG		25	3.471	46.326	37.218	1.00 39.65	A
ATOM	212	NE	ARG	A	25	4.873	45.907	37.177	1.00 40.74	A
ATOM	213	CZ	ARG	A	25	5.308	44.687	37.496	1.00 43.06	A
ATOM	214	NH1	ARG	A	25	4.453	43.749	37.885	1.00 39.85	A
ATOM	215	NH2	ARG	A	25	6.606	44.399	37.399	1.00 40.30	A
ATOM	216	C	ARG	A	25	2.590	48.270	32.651	1.00 28.86	A
ATOM	217	0	ARG	A	25	1.907	49.296	32.728	1.00 29.35	A
ATOM	218	N	ILE	Α	26	3.587	48.147	31.790	1.00 25.96	A
ATOM	219	CA	ILE	A	26	3.917	49.226	30.875	1.00 29.07	A
ATOM	220	CB	ILE		26	5.132	48.832	29.990	1.00 28.43	A
ATOM	221	CG2	ILE	A	26	5.239	49.760	28.799	1.00 25.38	A
ATOM	222	CG1			26	6.414	48.835	30.839	1.00 28.70	A
ATOM	223	CD1			26	7.546	48.257	3C.132	1.00 27.77	A
ATOM	224	C	ILE		26	2.719	49.571	29.968	1.00 30.92	A
MOTA	225	0	ILE		26	2.435	50.746	29.690	1.00 32.33	A
ATOM	226		LYS		27	2.019	48.540	29.512	1.00 30.36	A
ATOM	227		LYS		27	0.887	48.730	28.627	1.00 30.40	A
ATOM	228		LYS		27	0.449	47.388	28.045	1.00 33.83	A
ATOM	229		LYS		27	1.520	46.729	27.185	1.00 39.64	A
ATOM	230		LYS		27	1.167	45.294	26.831	1.00 44.41	A
ATOM	231	CE	LYS	Ä	27	-0.086	45.204	25.003	1.00 46.84	A

Figure 11D

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

MOTA	232	NZ	LYS	A	27	-0.384	43.774	25.598	1.00 53.94	A
ATOM	233	C		Ą	27	-0.267	49.402	29.344	1.00 28.67	A
ATOM	234	0		A	27	-0.919	50.252	28.767	1.00 26.05	A
	235	N	LYS	A	28	-0.511	49.020	30.593	1.00 27.68	A
ATOM					28	-1.597	49.609	31.371	1.00 27.30	A
MOTA	236	CA		À						
ATOM	237	CB		A	28	-1.797	48.845	32.691	1.00 24.82	A
ATOM	238	CG	LYS		28	-2.961	49.384	33.573	1.00 27.48	A
MOTA	239	$^{\circ}$	LYS	A	28	-4.263	49.506	32.744	1.00 31.59	A
ATOM	240	CE	LYS	Α	28	-5.526	49.699	33.606	1.00 30.02	A
ATOM	241	NZ	LYS	A	28	-5.440	50.820	34.586	1,00 31.11	A
ATOM	242	С	LYS	Α	28	-1.284	51.076	31.641	1.00 29.57	A
ATOM	243	0	LYS	Α	28	-2.164	51.951	31.566	1.00 28.21	A
ATOM	244	N	LEU		29	-0.017	51.359	31.923	1.00 29.36	A
ATOM	245	CA	LEU		29	0.385	52.723	32.179	1.00 33.70	A
ATOM	246	CB	LEU		29	1.822	52.745	32.692	1.00 35.26	A
		CG	LEU		29	2.023	53.727	33.847	1.00 38.04	A
ATOM	247						53.485	34.506	1.00 39.85	A
ATOM	248	CDl	LEU		29	3.363				
ATOM	249	CD2	LEU		29	1.891	55.149	33.332	1.00 38.01	A
ATOM	250	C	LEU		29	0.243	53.561	30.905	1.00 34.59	A
ATOM	251	0	LEU	A	29	-0.281	54.691	30.927	1.00 37.16	A
ATOM	252	N	LEU	A	30	0.721	53.020	29.792	1.00 34.03	A
MOTA	253	CA	LEU	Α	30	0.616	53.724	28.528	1.00 35.56	A
ATOM	254	CB	LEU	A	30	1.230	52.874	27.414	1.00 38.09	A
ATOM	255	CG	LEU	A	30	1.470	53.508	26.050	1.00 40.19	A
ATOM	256	CD1	LEU	A	30	2.270	54.805	26.163	1.00 39.79	A
ATOM	257	CD2	LEU		30	2.215	52.484	25.198	1.00 45.44	A
ATOM	258	C	LEU		30	-0.882	53.980	28.263	1.00 34.76	A
ATOM	259	ō	LEU		30	-1.269	55.050	27.794	1.00 33.56	A
ATOM	260	N	GLN		31	-1.713	52.996	28.572	1.00 30.55	A
					31	-3.152	53.142	28.401	1.00 31.04	A
ATOM	261	CA	GLN GLN		31	-3.865	51.839	28.782	1.00 31.04	A
ATOM	262	CB								
ATOM	263	CG	GLN		31	-5.397	51.924	28.839	1.00 37.09	A
ATOM	264	CD	GLN		31	-6.045	50.582	29.159	1.00 45.53	A
ATOM	265	OE1	GLN		31	-5.715	49.940	30.159	1.00 52.72	A
ATOM	266	NE2	GLN		31	-6.973	50.151	28.310	1.00 46.91	A
ATOM	267	C	GLN	A	31	-3.633	54.303	29.273	1.00 31.34	A
ATOM	268	С	GLN	Α	31	-4.419	55.125	28.832	1.00 28.45	A
MOTA	269	N	LEU	A	32	-3.141	54.376	30.509	1.00 30.93	A
ATOM	270	CA	LEU	A	32	-3.523	55.459	31.393	1.00 30.83	A
ATOM	271	CB	LEU	A	32	-2.988	55 237	32.811	1.00 29.49	A
ATOM	272	CG	LEU	A	32	-3.572	54.156	33.732	1.00 31.79	A
ATOM	273	CD1	LEU	Α	32	-2.810	54.215	35.075	1.00 33.29	A
ATOM	274	CD2		A	32	-5.058	54.376	33.972	1.00 25.39	A
ATOM	275	C	LEU		32	-3.031	56.797	30.850	1.00 32.26	A
ATOM	276	0		A	32	-3.707	57.810	31.031	1.00 35.77	A
	277	N	THR		33	-1.872	56.798	30.198	1.00 31.70	A
ATOM		CA	THR		33	-1.298	58.019	29.640	1.00 33.33	A
ATOM	278				33	0.158	57.787	29.156	1.00 35.07	A
ATOM	279	CB	THR						1.00 39.00	A
ATOM	280	OG1	THR		33	0.949	57.272	30.238		
ATOM	281		THR		33	0.776	59.087	28.687	1.00 34.58	A
ATOM	282	С	THR		33	-2.120	58.560	28.471	1.00 33.63	A
ATOM	283	0	THR		33	-2.237	59.767	28.298	1.00 33.87	A
MOTA	284	N	VAL	Α	34	-2.682	57.660	27.670	1.00 35.32	A
ATOM	285	CA	VAL	A	34	-3.507	58.046	26.531	1.00 36.90	A
ATOM	286	CB	VAL	A	34	-3.810	56.832	25,622	1.00 36.47	A
ATOM	287	CG1	VAL		34	-4.825	57.200	24.550	1.00 34.36	A
ATOM	288	CG2	VAL		34	-2.514	56.354	24.966	1.00 38.97	A
ATOM	289	С	VAL		34	-4.809	58.655	27.036	1.00 37.01	A
MOTA	290	ō	VAL		34	-5.250	59.695	26.540	1.00 35.59	A
ATOM	291	N	TRP		35	-5.403	57.992	28.022	1.00 36.34	A
A1011			- 1/1			2.200				

Figure I1E

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

MOTA	292	CA	TRP A	3.5	-6.645	58.429	28.648	1.00 38.95	A
MOTA	293	CB	TRP A	. 35	-7.022	57.429	29.742	1.00 44.03	A
ATOM	294	CG	TRP A	. 35	-8.302	57 716	30.478	1.00 45.10	A
ATOM	295	CD2	TRP A		-8.445	58.535	31.640	1.00 46.19	A
ATOM	296	CE2	TRP A	. 35	-9.820	58.545	31.973	1.00 47.39	A
ATOM	297	CE3	TRP A	. 35	-7.556	59.277	32.429	1.00 46.15	A
ATOM	298	CD1	TRP A	. 35	-9.549	57.260	30.166	1.00 45.42	A
MOTA	299	NE l	TRP A	. 35	-10.468	57.752	31.063	1.00 47.75	A
ATOM	300	CZ2	TRP A	. 35	-10.317	59.258	33.067	1.00 48.12	A
ATOM	301	CZ3	TRP A	. 35	-8.049	59.991	33.509	1.00 44.34	A
MOTA	302	CH2	TRP A	. 35	-9.419	59.968	33.824	1.00 47.03	A
ATOM	303	С	TRP A	. 35	-6.408	59.814	29.259	1.00 40.04	A
ATOM	304	0	TRP A	. 35	-7.155	60.759	29.013	1.00 39.15	A
ATOM	305	N	GLY A	. 36	-5.352	59.934	30.055	1.00 38.98	A
ATOM	306	CA	GLY A	. 36	-5.039	61.211	30.658	1.00 38.44	A
ATOM	307	С	GLY A	. 36	-5.034	62.327	29.634	1.00 38.41	A
ATOM	308	0	GLY A	36	-5.626	63.390	29.845	1.00 40.58	A
ATOM	309	N	ILE A	. 37	-4.356	62.094	28.517	1.00 39.01	A
ATOM	310	CA	ILE A	. 37	-4.279	63.079	27.451	1.00 40,60	A
MOTA	311	CB	ILE A	. 37	-3.395	62.584	26.301	1.00 40.20	A
ATOM	312	CG2	ILE A	. 37	-3.509	63.517	25.136	1.00 39.97	A
MOTA	313	CG1	ILE A	. 37	-1.939	62.477	26.767	1.00 41.25	A
MOTA	314	CD1	ILE A	37	-1.036	61.777	25.778	1.00 38.31	A
ATOM	315	C	ILE A	. 37	-5.662	63.366	26.886	1.00 42.00	A
ATOM	316	0	ILE A	37	-6.019	64.516	26.654	1.00 42.52	A
ATOM	317	N	LYS A	38	-6.438	62.317	26.660	1.00 42.56	A
ATOM	318	CA	LYS A	38	-7.766	62.505	26.112	1.00 45.16	A
ATOM	319	CB	LYS A	38	-8.459	61.156	25.925	1.00 46.50	A
ATOM	320	CG	LYS A	38	-9.683	61.235	25.026	1.00 53.52	A
ATOM	321	CD	LYS A	38	-10.840	62.017	25.651	1.00 55.55	A
ATOM	322	CE	LYS A	38	-11.812	62.480	24.581	1.00 56.01	A
ATOM	323	NZ	LYS A	38	-11.165	63.504	23.714	1.00 55.27	A
ATOM	324	C	LYS A	38	-8.594	63.405	27.025	1.00 46.34	A
ATOM	325	0	LYS A		-9.237	64.343	26.561	1.00 48.52	A
ATOM	326	N	GLN A	39	-8.554	63.120	28.322	1.00 47.82	A
ATOM	327	CA	GLN A	39	-9.303	63.877	29.318	1.00 49.21	A
ATOM	328	CB	GLN A	39	-9.142	63.230	30.591	1.00 52.07	A
ATOM	329	CG	GLN A	39	-9.431	61.742	30.727	1.00 59.01	A
ATOM	330	CD	GLN A	39	-10.889	61.409	30.513	1.00 61.01	A
MOTA	331	OE1		39	-11.742	61.800	31.310	1.00 63.56	A
MOTA	332	NE2	GLN A	39	-11.188	60.677	29.437	1.00 62.00	A
MOTA	333	С	GLN A	39	-8.840	65.324	29.412	1.00 48.78	A
MOTA	334	0	GLN A	39	-9.649	66.243	29.431	1.00 48.03	A
ATOM	335	N	LEU A	40	-7.530	65.522	29.472	1.00 49.67	A
ATOM	336	CA	LEU A	40	-6.980	66.861	29.590	1.00 50.78	A
ATOM	337	CB	LEU A	40	-5.479	66.785	29.868	1.00 49.62	A
ATOM	338	CG	LEU A	40	-4.736	68.118	29.982	1.00 47.99	A
ATOM	339	CD1	LEU A	40	-5.416	69.030	31.011	1.00 51.32	A
MOTA	340		LEU A	40	-3.300	67.852	30.376	1.00 48.82	A
ATOM	341	C	LEU A	40	-7.227	67.736	28.363	1.00 53.20	A
ATOM	342	0	LEU A	40	-7.230	68.964	28.457	1.00 53.67	A
MOTA	343	И	GLN A	41	-7.433	67.104	27.215	1.00 56.61	A
ATOM	344	CA	GLN A	41	-7.649	67.850	25.994	1.00 60.81	A
ATOM	345	CB	GLN A	41	-7.295	66.994	24.781	1.00 60.00	A
ATOM	346	CG	GLN A	41	-7.257	67.753	23.467	1.00 61.60	A
ATOM	347	CD	GLN A	41	-6.756	66.885	22.330 22.367	1.00 61.14	A.
ATOM	348		GLN A	41	-5.630	66.377	22.367	1.00 56.12	A
ATOM	349			41 41	-7.598 -9.084	66.697	25.915	1.00 60.61	A
MOTA MOTA	350 351	0	GLN A GLN A		-9.388	68.344 69.277	25.179	1.00 63.54 1.00 65.13	A A
AL ON	ند ل	J	ATTA M	41	-5.500	00.277	لا ۱ شد . ب بد	1.00 00.10	

Figure 11F

MOTA	352	M	ALA	A	42	-9.971	67.722	26.679	1.00 67.16	A
ATOM	253	CA	ALA	A	42	-11.362	68.150	26.693	1.00 70.08	A
MOTA	354	CB	ALA	A	42	-12.252	67.043	27.249	1.00 68.59	A
ATOM	355	С	ALA	Α	42	-11.461	69.423	27.556	1.00 72.76	A
ATOM	356	0	ALA	A	42	-12.506	69 748	28.123	1.00 73.45	A
ATOM	357	N	ARG	Α	43	-10.338	70.137	27.642	1.00 75.35	A
ATOM	358	CA	ARG	A	43	-10.202	71.377	28.413	1.00 76.97	A
ATOM	359	CB	ARG	A	43	-9.391	71.131	29.705	1.00 77.23	A
ATOM	360	CG	ARG	Α	43	-10.130	70.250	30.753	1.00 77.83	A
ATOM	361	$\mathbb{C}\mathbb{D}$	ARG	A	43	-9.265	69.690	31.889	1.00 76.18	A
ATOM	362	NE	ARG	A	43	-10.053	68.919	32.864	1.00 76.19	A
ATOM	363	CZ	ARG	Α	43	-10.933	67.967	32.551	1.00 76.17	A
MOTA	364	NH1	ARG	A	43	-11.153	67.657	31.284	1.00 76.24	A
ATOM	365	NH2	ARG	A	43	-11.605	67.326	33.507	1.00 77.89	A
ATOM	366	С	ARG	A	43	-9.560	72.481	27.570	1.00 79.19	A
ATOM	367	0	ARG	A	43	~10.131	72.882	26.548	1.00 79.42	A
ATOM	368	N	ILE	A	44	-8.381	72.970	27.993	1.00 81.42	A
ATOM	369	CA	ILE	A	44	-7.646	74.059	27.276	1.00 84.32	A
ATOM	370	CB	ILE	A	44	-6.073	73.998	27.495	1.00 84.97	A
MOTA	371	CG2	ILE		44	-5.292	74.824	26.419	1.00 85.80	A
ATOM	372	CG1	ILE		44	-5.728	74.612	28.829	1.00 85.52	A
ATOM	373		ILE		44	-6.344	76.011	29.055	1.00 87.04	A
ATOM	374	С	ILE		44	-7.908	73.987	25.790	1.00 86.80	A
ATOM	375	0	ILE		44	-8.577	74.829	25.234	1.00 87.60	A
ATOM	376	N	LEU		4.5	-7.318	73.007	25.145	1.00 87.99	A
ATOM	377	CA	LEU		45	-7.541	72.910	23.737	1.00 88.13	A
ATOM	378	CB	LEU		45	-6.257	72.509	23.009	1.00 88.79	A
MOTA	379	CG		A	45	-5.940	73.339	21.770	1.00 90.46	A
ATOM	380		LEU		45	-7.147	73.370	20.837	1.00 91.58	A
ATOM	381		LEU		45	-5.596 -8.656	74.779 71.944	22.173	1.00 90.84	A
ATOM ATOM	382 383	0	LEU		45 45	-8.636 -9.507	71.665	23.376 24.291	1.00 88.30 1.00 87.82	A A
ATOM	384	NI	LEU		45	-8.614	71.561	22.151	1.00 88.77	A A
ATOM	385	CA		В	0	29.175	18.175	21.874	1.00 35 90	B
ATOM	386	C		B	0	27.867	18.849	22.146	1.00 36 69	B
ATOM	387	ō	ACE		0	27.836	20.078	22.299	1.00 33.24	В
ATOM	388	N	ARG		1	26.771	18.065	22.218	1.00 32 69	B
ATOM	389	CA	ARG		1	25.440	18.590	22.450	1.00 34.24	В
ATOM	390	CB	ARG		1	24.436	17.446	22.644	1.00 33.49	В
ATOM	391	CG	ARG		1	22.976	17.878	22.651	1.00 32.92	В
ATOM	392	CD	ARG	B	1	22.436	18.177	21.260	1.00 34.95	В
ATOM	393	NE	ARG	B	1	22.366	16.972	20.443	1.00 38.88	B
MOTA	394	CZ	ARG	3	1	21.548	15.952	20.706	1.00 42.79	B
ATOM	395	NH1	ARG	В	1	20.740	16.012	21.765	1.00 44.65	B
ATOM	396	NH2	ARG	В	1	21.550	14.868	19.943	1.00 39.72	B
ATOM	397	C	ARG	В	1	25.424	19.498	23.685	1.00 35.96	B
ATOM	398	0	ARG	В	1	24.920	20.617	23.628	1.00 36.55	В
ATOM	399	N		В	2	26.008	19.009	24.779	1.00 39.89	B
ATOM	400	CA		В	2	26.077	19.769	26.022	1.00 43.08	B
ATOM	401	CB		В	2	27.113	19.163	26.972	1.00 43.87	В
ATOM	402	CG	MET		2	26.728	17.847	27.623	1.00 46.86	В
ATOM	403	SD	MET		2	25.304	18.010	28.700	1.00 52.01	В
ATOM	404	CE	MET		2	24.024	18.375	27.524	1.00 52.70	В
ATOM	405	С	MET		2	26.440	21.219	25.789	1.00 45.76	В
MOTA	406 407	0	MET		2	25.723 27.570	22.121	26.212	1.00 44.09 1.00 47.94	3
MOTA MOTA	407	N CV	LYS		3	28.082	21.414 22.736	25.125 24.820	1.00 4,.94	В
ATOM	409	CA CB	LYS		3 3	28.082	22.736	24.820	1.00 52.42	B B
ATOM	410	CG	LYS		3	30.552	23.540	24.595	1.00 58.36	a B
ATOM	411	CD	LYS		3	30.382	24.937	24 030	1.00 60.17	B
				_	~	50.505	- 1 - 2 2 /	050	2.00 00.17	

Figure 11G

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

MOTA	412	CE	LYS	В	3	31.61	8 25.777	24.321	1.00 62.06	В
ATOM	413	NZ	LYS	В	3	31.56	27.140	23.704	1.00 63.71	В
ATOM	414	С	LYS	В	3	27.09		23.907	1.00 52.65	B
ATOM	415	0	LYS	В	3	26.85	8 24.671	24.092	1.00 52.44	₿
MOTA	416	13	GLN	В	4	26.51	7 22.774	22.934	1.00 52.13	B
ATOM	417	CA	GLN	В	4	25.549	9 23.387	22.032	1.00 54.04	В
ATOM	418	CB	GLN	В	4	24.930	22.330	21.105	1.00 57.72	B
MOTA	419	CG	GLN	B	4	25.792	2 21.880	19.925	1.00 60.44	B
ATOM	420	CD	GLN	В	4	25.85	5 22.923	18.816	1.00 62.71	B
MOTA	421	OE1	GLN	B	4	26.404	24.017	18.997	1.00 64.51	В
ATOM	422	NE2	GLN	₿	4	25.276	32.592	17.661	1.00 62.62	₿
MOTA	423	С	GLN	В	4	24.44	24.062	22.836	1.00 52.63	В
ATOM	424	0	GLN	В	4	24.013	25.162	22.518	1.00 53.56	В
ATOM	425	N	ILE	В	5	23.982	23.379	23.878	1.00 52.62	В
MOTA	426	CA	ILE	В	5	22.929	23.880	24.758	1.00 52.43	B
ATOM	427	CB	ILE	В	5	22.443	3 22.766	25.721	1.00 51.17	В
ATOM	428	CG2	ILE	В	5	21.412	23.329	26.691	1.00 52.10	В
MOTA	429	CG1	ILE	В	5	21.871	21.592	24.917	1.00 52.55	B
MOTA	430	CD1	ILE	В	5	21.496	20.363	25.754	1.00 53.47	В
ATOM	431	C	ILE	В	5	23.452	25.043	25.600	1.00 53.54	В
MOTA	432	0	ILE	В	5	22.743	26.013	25.849	1.00 52.58	В
MOTA	433	N	GLU	В	6	24.701	24.932	26.036	1.00 55.54	В
ATOM	434	CA	GLU	В	6	25.309	25.970	26.850	1.00 56.11	В
ATOM	435	CB	GLU	В	6	26.637	25.477	27.437	1.00 53.75	В
MOTA	436	CG	GLU	В	б	26.487	24.157	28.171	1.00 53.07	В
ATOM	437	CD	GLŲ	В	6	27.729	23.735	28.939	1.00 50.56	В
ATOM	438	OE1	GLU	В	6	28.816	23.611	28.329	1.00 49.24	В
ATOM	439	OE2	GLU	В	6	27.604	23.516	30.159	1.00 47.31	В
ATOM	440	С	GLU	В	6	25.522	27.217	26.009	1.00 57.04	B
ATOM	441	0	GLU	В	6	25.418	28.335	26.515	1.00 58.94	В
ATOM	442	N	ASP	В	7	25.811	27.031	24.725	1.00 57.18	В
MOTA	443	CA	ASP	В	7	26.003	28.179	23.848	1.00 58.51	В
ATOM	444	CB	ASP	В	7	26.681	27.772	22.536	1.00 59.88	В
ATOM	445	CG	ASP	В	7	28.121	27.339	22.732	1.00 62.42	B
MOTA	445	OD1	ASP	В	7	28.827	27.979	23.542	1.00 62.53	B
ATOM	447	002	ASP	В	7	28.559	26.382	22.056	1.00 66.19	В
ATOM	448	С	ASP	В	7	24.668	28.858	23.543	1.00 58.25	B
ATOM	449	0	ASP	В	7	24.624	30.070	23.314	1.00 56.00	B
ATOM	450	N	LYS	В	8	23.591		23.547	1.00 57.96	B
ATOM	451	CA	LYS	В	8	22.240	28.563	23.276	1.00 57.58	В
ATOM	452	CB	LYS	В	8	21.331	27.405	22.838	1.00 57.99	В
MOTA	453	CG	LYS	В	8	19.911	27.844	22.484	1.00 60.08	В
ATOM	454	CD	LY5	B	8	19.915	28.785	21.280	1.00 60.12	В
ATOM	455	CE	LYS	В	8	18.697	29.725	21.268	1.00 60.76	В
ATOM	456	NZ	LYS	В	8	17.371	29.062	21.146	1.00 58.46	B
ATOM	457	C	LYS	В	8	21.653	29.248	24.517	1.00 56.86	B
MOTA	458	0	LYS	В	8	20.832	30.166	24.411	1.00 53.70	В
ATOM	459	N	ILE	В	9	22.077	28.790	25.689	1.00 57.87	В
ATOM	460	CA	ILE	В	9	21.621	29.368	26.947	1.00 59.31	В
ATOM	461	CB	ILE	В	9	22.073	28.517	28.161	1.00 57.40	₿
ATOM	462	CG2	ILE	В	9	21.788	29.270	29.459	1.00 57.21	B
MOTA	463	CGl	ILE	В	9	21.361	27.165	28.154	1.00 56.21	B
ATOM	464	CDl	ILE		9	21.885	26.199	29.212	1.00 54.49	B
ATOM	465	С	ILE	₿	9	22.216	30.770	27.093	1.00 60.74	B
MOTA	466	0	ILE	В	9	21.565	31.682	27.608	1.00 61.51	В
atom	467	N	GLU	3	10	23.456	30.923	26.633	1.00 61.69	В
ATOM	468	CA	GLU	В	10	24.170	32.198	26.691	1.00 63.76	В
MOTA	469	CB	GLU	3	10	25.629	32.000	26.279	1.00 63.63	В
MOTA	470	CG	GLU		10	26 456	33.275	26.254	1,00 65.58	B
ATOM	471	CD	GLU	B	10	27.854	33.054	25.707	1.00 66.48	В

Figure 11H

ATOM	472		GLU		10	27.979	32.751	24.499	1.00 67.38	3
MOTA	473	OE2			LO	28.824	33.173	26.485	1.00 66.28	В
ATOM	474	С	GLU		L 0	23.515	33.211	25.757	2.00 65.16	В
ATOM	475	0	GLU		LO	23.261	34.351	26.141	1.00 65.81	В
ATOM	476	N	GLU	B :	L1	23.255	32.785	24.524	1.00 66.64	В
ATOM	477	CA	GLU	В :	11	22.517	33.637	23.529	1.00 67.59	В
ATOM	478	CB	GLU		.1	22.348	32.832	22.252	1.00 68.72	В
ATOM	479	CG	GLU	В :	.1	21.735	33.636	21.117	1.00 72.88	В
ATOM	480	CD	GLU	В :	.1	22.556	34.864	20.767	1.00 74.80	В
ATOM	481	OE1	GLU	B :	.1	23.775	34.717	20.526	1.00 75.81	B
ATOM	482	OE2	GLU	В :	. 1	21.978	35.975	20.731	1.00 74.99	В
ATOM	483	C	GLU	В 3	.1	21.307	34.197	24.098	1.00 67.17	В
ATOM	484	0	GLU	B 3	.1	20.998	35.381	23.918	1.00 68.06	В
ATOM	485	N	ILE	В 3	.2	20.541	33.348	24.784	1.00 64.61	В
MOTA	486	CA	ILE	B 1	.2	19.288	33.790	25.389	1.00 61.65	В
ATOM	487	CB	ILE	B 1	.2	18.458	32.600	25,926	1.00 62.84	В
ATOM	488	CG2	ILE	B 1	.2	17.416	33.094	26.940	1.00 62.63	B
ATOM	489	CGl	ILE	B 3	.2	17.799	31.864	24.750	1.00 62.13	В
ATOM	490	CD1	ILE	В 3	.2	16.910	30.698	25.156	1.00 61.39	В
ATOM	491	С	ILE	В 1	2	19.553	34.776	26.522	1.00 58.17	В
ATOM	492	0	ILE	B 1	2	19.010	35.881	26.523	1.00 55.05	В
ATOM	493	N	GLU	B 1	.3	20.388	34.384	27.479	1.00 55.87	B
ATOM	494	CA	GLU	B 1	3	20.710	35.268	28.600	1.00 54.71	В
ATOM	495	CB	GLU	B 1	.3	21.817	34.669	29.477	1.00 50.19	В
ATOM	496	CG	GLU	B 1	3	21.447	33.331	30.109	1.00 49.30	B
ATOM	497	CD	GLU	в 1	3	22.577	32.729	30.933	1.00 49.10	B
MOTA	498	OE1	GLU		3	23.741	32.765	30.472	1.00 50.79	B
ATOM	499	OE2	GLU	в 1	3	22.304	32.194	32.027	1.00 47.00	B
ATOM	500	С	GLU	B 1	3	21.166	36.612	28.047	1.00 55.57	В
ATOM	501	0	GLU	в 1	3	20.790	37.667	28.557	1.00 56.33	В
ATOM	502	N	SER		4	21.950	36.559	26.977	1.00 56.02	В
ATOM	503	CA	SER	В 1	4	22.468	37.763	26.350	1.00 55.71	В
MOTA	504	CB	SER	В 1	4	23.488	37.389	25.278	1.00 54.62	В
ATOM	505	QG	SER	в 1	4	23.968	38.550	24.629	1.00 56.74	В
ATOM	506	С	SER	B 1	4	21.366	38.624	25.736	2.00 55.96	В
ATOM	507	0	SER	B 1	4	21.459	39.854	25.696	1.00 54.91	В
ATOM	508	N	LYS	B 1	5	20.310	37.979	25.263	1.00 55.94	B
ATOM	509	CA	LYS	B 1	5	19.208	38.704	24.650	1.00 56.72	В
ATOM	510	CB	LYS :	в 1	5	18.454	37.779	23.693	1.00 55.67	В
MOTA	511	CG	LYS :	B 1	5	17.494	38.484	22.772	1.00 58.33	В
ATCM	512	CD	LYS I	B 1	5	17,000	37.527	21.705	1.00 59.89	B
ATOM	513	CE	LYS I	в 1	5	16.440	38.282	20.518	1.00 60.44	В
ATOM	514	NZ	LYS :	в 1	5	16.020	37.375	19.412	1.00 63.67	В
MOTA	515	C	LYS I	B 1	5	18.282	39.207	25.748	1.00 56.31	B
ATOM	516	0	LYS :	B 1	5	17.716	40.296	25.661	1.00 56.65	B
ATOM	517	N	GLN :	B 1	5	18.146	38.403	26.791	1.00 56.76	B
MOTA	518	CA	GLN 1	В 1	5	17.293	38.748	27.911	1.00 57.28	B
ATOM	519	CB	GLN I	В 1	5	17.306	37.604	28.923	1.00 56.94	В
MOTA	520	CG	GLN I	B 1	5	16.000	37.394	29.652	1.00 55.90	В
ATOM	521	CD	GLN I	B 1	5	15.908	36.017	30.300	1.00 56.24	B
ATOM	522	OE1	GLN I	B 1	5	16.613	35.722	31.263	1.00 57.78	В
ATOM	523	NE2	GLN R	B 1	5	15.044	35.160	29.760	1.00 55.69	В
ATOM	524	C	GLN E	8 1	5	17.825	40.040	28.528	1.00 58.82	В
ATOM	525	0	GLN E	3 1	5	17.049	40.929	28.905	1.00 59.68	В
ATOM	526	N	LYS E	в 1.	7	19.148	40.163	28.621	1.00 59.44	3
ATOM	527	CA	LYS E	3 1	7	19.711	41.379	29.189	1.00 59.84	В
ATOM	528	CB	LYS E			21.228	41.275	29.386	1.00 60.80	B
ATOM	529	CG	LYS E		7	21.740	42.343	30.356	1.00 64.52	B
ATOM	530	CD	LYS E	3 1	7	23.250	42.325	30.576	1.00 65.30	B
MOTA	531	CE	LYS E		7	24.008	42.784	29.344	1.00 67.22	B
										_

Figure 11I

MOTA	532	NZ	LYS	В	17	25 465	42.963	29.625	1.00 67.09	В
MOTA	533	С	LYS	В	17	19.389	42.522	28.230	1.00 59.16	В
ATOM	534	0	LYS		17	19.388	43.634	28,656	1.00 55.77	В
ATOM	535	N	LYS		18	19.433	42.233	26.931	1.00 58.38	B
ATOM	536	ÇA	LYS	В	18	19.128	43.248	25.931	1.00 58.35	В
MOTA	537	CB	LYS		18	19.247	42.675	24.511	1.00 59.38	B
ATOM	538	CG	LYS	В	18	20.617	42.083	24.130	1.00 61.47	В
ATOM	539	CD	LYS		18	21.768	43.111	24.099	1.00 51,91	В
ATOM	540	CE	LYS	В	18	22.034	43.761	25.461	1.00 63,50	B
MOTA	541	NZ	LYS	В	18	23.248	44.620	25.423	1.00 63.66	B
MOTA	542	С	LYS	В	18	17.706	43.761	26.163	1.00 58,27	В
ATOM	543	0	LYS	В	18	17.475	44.969	26.254	1.00 58,82	B
ATOM	544	N	ILE		19	16.757	42.835	26.268	1.00 56.89	В
ATOM	545	CA	ILE		19	15.356	43.189	26.488	1.00 53.76	B
MOTA	546	CB	ILE		19	14.455	41.931	26.488	1.00 53.33	B
ATOM	547	CG2	ILE		19	13.057	42.286	26.976	1.00 52.66	В
ATOM	548	CG1	ILE		19	14.416	41.322	25.081	1.00 52.79	B
ATOM	549	CD1	ILE		19	13.543	40.069	24.970	1.00 54.45	B
ATOM	550	С	ILE		19	15.117	43.961	27.786	1.00 52,88	В
MOTA	551	0	ILE		19	14.327	44.897	27.809	1.00 51.74	В
ATOM	552	N	GLU		20	15.781	43.565	28.869	1.00 51.04	B
ATOM	553	CA	GLU		20	15.601	44.267	30.128	1.00 50.08	B
ATOM	554	CB	GLU		20	16.403	43.613	31.253	1.00 49.90	В
MOTA	555	CG	GLU		20	15.969	42.207	31.584	1.00 54.19	B
ATOM	556	CD	GLU		20	16.761	41.620	32.736	1.00 55.98	B
ATOM	557	OE1	GLU		20	18.010	41.568	32.641	1.00 53.23	В
ATOM	558	OE2	GLU		20	16.127	41.215	33.735	1.00 56.20	В
ATOM ATOM	559 560	0			20 20	16.053 15.479	45.706	29.965	1.00 49.26	В
ATOM	561	N	GLU ASN		21	17.093	46.611 45.912	30.561	1.00 48.88	В
ATOM	562	CA	ASN		21	17.596	47.256	28.930	1.00 49.15	B
ATCM	563	CB	ASN		21	18.885	47.229	28.098	1.00 49.99	B B
MOTA	564	CG	ASN		21	20.054	46.576	28.834	1.00 54.79	В
ATOM	565		ASN		21	20.421	46.978	29.943	1.00 55.96	В
ATOM	566		ASN		21	20.656	45.572	28.205	1.00 57.15	В
ATOM	567	C	ASN		21	16,537	48.078	28.202	1.00 49.83	B
ATOM	568	0	ASN		21	16.249	49.209	28.591	1.00 50.14	В
ATOM	569	N	GLU	B	22	15.957	47.497	27.153	1.00 47.34	В
ATOM	570	CA	GLU	В	22	14.942	48.160	26.354	1.00 44.99	В
ATOM	571	СЭ	GLU	В	22	14.534	47.272	25.174	1.00 44.99	В
ATOM	572	CG	GLU	В	22	13.703	47.990	24.116	1.00 51.85	В
MCTA	573	CD	GLU	В	22	14.377	49.268	23.621	1.00 54.71	В
ATOM	574	OE1	GLU	B	22	15.543	49.191	23.182	1.00 55.60	В
ATOM	575	OE2	GLU	В	22	13.743	50.350	23.673	1.00 57.01	В
ATOM	576	C	GLU	В	22	13.710	48.521	27.183	1.00 44.17	B
ATOM	577	0	GLU	В	22	13.044	49.527	26.916	1.00 45.50	B
ATOM	578	N	ILE	В	23	13.386	47.693	28.169	1.00 42.28	3
ATOM	579	CA	ILE	В	23	12.241	47.977	29.024	1.00 40.61	В
ATOM	580	CB	ILE		23	11.801	46.724	29.809	1.00 38.57	${\mathtt B}$
ATOM	581	CG2	ILE		23	10.836	47.096	30.925	1.00 37.31	B
MOTA	582	CG1			23	11.138	45.733	28.850	1.00 38.28	В
ATOM	583	CD1			23	10.634	44.436	29.530	1.00 38.32	В
ATOM	584	C	ILE		23	12.626	49.108	29.974	1.00 41.50	В
ATOM	585	0	ILE		23	11.793	49.926	30.349	1.00 41.54	В
MOTA	586	N	ALA		24	13.898	49.170	30.348	1.00 40.42	В
ATOM	587	CA	ALA		24	14.349	50.240	31.224	1.00 38.49	В
ATOM	588 589	CB	ALA		24 24	15.811	50.059	31.578	1.00 34.26	B
ATOM ATOM	590	0	ALA ALA		24	14.147 13.674	51.562 52.528	30.490 31.078	1.00 37.76 1.00 38.39	В
ATOM	591	10	ARG		25	14.498	51.591	29.204	1.00 36.47	вя
AI OFI	ا ا ⊏ نہ	Y.A.	ت اکسید	Ð	40	14.470	٠-٠ ٢٣٠	-5.2U4	2.00 30.4/	3

Figure 11J

ATOM	592	CA	ARG	В	25	14.3	54	52.796	28.394	1.00 38.10	B
ATOM	593	CB	ARG	B	25	15.0	86	52.644	27.051	1.00 40.70	В
ATOM	594	CG	ARG	3	25	15.6	09	52.668	27.195	1.00 46.74	В
ATOM	595	CD	ARG	В	25	17.3	15	52.949	25.879	1.00 51.86	В
ATOM	596	NE	ARG	В	25	17.2	68	51.823	24.954	1.00 56.83	В
ATOM	597	CZ	ARG	B	25	17.8	94	50.666	25.152	1.00 59.56	B
MOTA	598	NHl	ARG	3	25	18.6	15	50.477	26.253	1.00 60.08	В
MOTA	599	NH2	ARG	В	25	17.7	92	49.696	24.257	1.00 59.81	В
ATOM	600	C	ARG	В	25	12.9	01	53.185	28.158	1.00 36.71	В
ATOM	601	0	ARG	В	25	12.5	55	54.361	28.165	1.00 36.54	В
ATOM	602	N	ILE	$\mathbf{B}$	26	12.0	51	52.197	27.942	1.00 36.23	В
MOTA	603	CA	ILE	В	26	10.6	42	52.454	27.733	1.00 34.33	В
MOTA	604	CB	ILE	В	26	9.9	44	51.152	27.370	1.00 34.16	B
ATOM	605	CG2			26	8.4	32	51.293	27.496	1.00 31.45	B
ATOM	606	CGl			26	10.43		50.722	25.985	1.00 34.01	В
ATOM	607	CD1			26	9.8		49.403	25.540	1.00 34.37	В
ATOM	608	С	ILE		26	10.04		53.059	29.005	1.00 34.32	В
ATOM	609	0	ILE		26	9.3		54.053	28.956	1.00 33.13	В
MOTA	610	N	LYS		27	10.3		52.457	30.141	1.00 34.59	В
MOTA	611	CA	LYS		27	9.89		52.941	31.433	1.00 35.31	В
MOTA	612	CB	LYS		27	10.36		52.005	32.544	1.00 36.43	В
ATOM	613	CG	LYS		27	9.39		50.872	32.885	1.00 40.24	В
ATOM	614	CD	LYS		27	10.18		49.643	33.347	1.00 44.60	В
ATOM	615	CE	LYS		27	11.27		49.991	34.334	1.00 50.65	В
ATOM	616	NZ	LYS		27	12.20		48.831	34.560	1.00 54.97	В
ATOM	617	C	LYS		27	10.38		54.355	31.712	1.00 35.58	В
ATOM	618	0	LYS		27	9.66		55.140	32.318	1.00 36.82	В
ATOM	619 620	N	LYS		28	11.59		54.670	31.268	1.00 36.91	B
ATOM ATOM	621	CA CB	LYS		28 28	12.18		55.993	31.463	1.00 37.71	В
	622		LYS			13.62		56.017	30.958	1.00 42.60	В
MOTA MOTA	623	CG CD	LYS		28 28	14.60 15.29		56.755 55.778	31.851 32.818	1.00 49.26	В
ATOM	624	CE	LYS		28	14.31		54.979	33.680	1.00 55.52	B
ATOM	625	NZ	LYS		28	15.01		53.887	34.421	1.00 59.10	B
ATOM	626	C	LYS		28	11.39		57.044	30.677	1.00 37.60	B B
ATOM	627	0	LYS		28	10.95		58.045	31.240	1.00 40.12	д В
ATOM	628	N	LEU		29	11.25		56.826	29.368	1.00 35.33	В
ATCM	629	CA	LEU		29	10.51		57.754	28.524	1.00 35.90	д В
ATOM	630	CB	LEU		29	10.44		57.267	27.071	1.00 36.49	B
ATOM	631	CG	LEU		29	9.49		58.127	26.202	1.00 37.58	B
MCTA	632	CDI	LEU		29	9.95		59.581	26.260	1.00 36.39	В
ATOM	633		LEU		29	9.44		57.641	24.744	1.00 35.00	B
ATOM	634	C	LEU		29	9.10		57.912	29.047	1.00 35.09	В
ATOM	635	0	LEU	В	29	8.56	8	59.015	29.095	1.00 34.76	В
ATOM	636	N	LEU	В	30	8.51	.2	56.787	29.426	1.00 33.74	В
ATOM	637	CA	LEU	В	30	7.16	1	56.746	29.946	1.00 30.65	В
ATOM	638	CB	LEU	В	30	6.78	9	55.284	30.181	1.00 32.72	В
ATOM	639	CG	LEU	В	30	5.38	5	54.822	30.558	1.00 31.65	B
MOTA	640	CD1	LEU	В	30	4.35	3 !	55.404	29.599	1.00 34.37	В
MOTA	641	CD2	LEU		30	5.37		53.282	30.511	1.00 31.69	В
ATOM	642	С	LEU	B	30	6.98	5	57.588	31.213	1.00 31.56	B
MOTA	643	0	LEU		30	ნ.05		58.398	31.301	1.00 26.54	B
MOTA	644	N	GLN		31	7.86			32.206	1.00 31.24	B
ATOM	645	CA	GLN		31	7.66			33.398	1.00 33.01	$\mathbb{B}$
MOTA	646	CB	GLN		31	8.55			34.564	1.00 33.79	В
ATOM	647	CG	GLN		31	10.01			34.321	1.00 40.81	В
ATOM	648	CD	GLN		31	10.73			35.491	1.00 44.04	В
ATOM	649		GLN		31	10.80		57.648	36.598	1.00 43.99	В
ATOM	650		GLN		31	11.27		55.889	35.258	1.00 41.97	В
MOTA	651	С	GLN	ם	31	7.90	0 :	59.734	33.072	1.00 34.12	В

Figure 11K

ATOM	652	0	GLN B	31	7.420	60.536	33.766	1 00 30.63	В
MOTA	653	N	LEU B	32	8.629	59.961	31.984	1.00 34.46	В
ATOM	654	CA	LEU B	32	8.935	61.292	31.523	1.00 36.10	В
ATOM	655	CB	LEU B	32	10.070	61.231	30.504	1.00 40.01	В
ATOM	656	ÇG	LEU B	32	10.340	62.546	29.775	1.00 40.15	3
ATOM	657	CD1		32	10.853	63.586	30 765	1.00 43.23	# B
ATOM	658	CD2		32	11.354	62.310	28.668	1.00 43.20	B
ATOM	659	C	LEU B	32	7.711	51.949	30.890	1.00 36.08	В
ATOM	660	0	LEU B	32	7.552	63.162	30.964	1.00 37.71	В
ATOM	661	N	THR B	33	6.859	61.149	30.255	1.00 32.40	В
MOTA	662	CA	THR B	33	5.659	61.679	29.617	1.00 31.31	B
ATOM	663	CB	THR B	33	5.179	60.753	28.480	1.00 30.70	В
ATOM	664	0G1		33	4.536	59.603	29.030	1.00 40.03	B
ATOM	665	CG2	THR B	33	6.371	60.282	27.654	1.00 31.28	₿
ATOM	666	С	THR B	33	4.550	61.845	30.668	1.00 30.03	B
ATOM	667	0	THR B	33	3.739	62.772	30.585	1.00 30.10	В
ATOM	668	N	VAL B	34	4.507	60.933	31.636	1.00 27.29	В
ATOM	669	CA	VAL B	34	3.546	61.010	32.735	1.00 25.28	3
ATOM	670	CB	VAL B	34	3.695	59.806	33.690	1.00 25.71	В
ATOM	671	CG1	VAL B	34	2.920	60.036	34.985	1.00 27.25	В
MOTA	672	CG2	VAL B	34	3.176	58.565	32.997	1.00 23.84	В
MOTA	673	C	VAL B	34	3.822	62.310	33.476	1.00 22.65	B
ATOM	674	ō	VAL B	34	2.899	63.064	33.763	1.00 21.36	В
MOTA	675	N	TRP B	35	5.100	62.580	33.757	1.00 22.24	В
MOTA	676	CA	TRP B	35	5.502	63.828	34.414	1.00 20.87	13 18
	677	CB	TRP B	35	7.016	63.843	34.653	1.00 23.71	В
MOTA MOTA				35	7.523		35.434		
	678	CG	TRP B			65.040			В
ATOM	679	CD2		35	7.013	65.551	36.681	1.00 25.13	В
ATOM	680	CE2	TRP B	35	7.767	66.698	37.003	1.00 28.35	В
MOTA	681	CE3		35	5.985	65.143	37.547	1.00 24.83	В
ATOM	682	CD1		35	8.540	65.880	35.074	1.00 25.67	B
MOTA	683	NE 1		35	8.692	66.877	36.006	1.00 27.74	В
ATOM	684	CZ2	TRP B	35	7.532	67.455	38.165	1.00 28.38	В
ATOM	685	CZ3	TRP B	35	5.749	65.889	38.699	1.00 23.47	B
ATOM	686	CH2	TRP B	35	6.516	67.034	38.999	1.00 28.31	В
ATOM	687	C	TRP B	35	5.121	65.039	33.564	1.00 24.26	В
ATOM	688	0	TRP B	35	4.695	66.063	34.088	1.00 23.94	В
ATOM	689	N	GLY B	36	5.308	64.927	32.247	1.00 25.59	В
ATOM	690	CA	GLY B	36	4.961	66.013	31.348	1.00 23.22	B
MOTA	691	C	GLY B	36	3.479	66.364	31.343	1.00 25.72	B
ATOM	692	0	GLY B	36	3.138	67.539	31.352	1.00 28.94	В
ATOM	693	N	ILE B	37	2.610	65.356	31.311	1.00 27.20	В
ATOM	694	CA	ILE B	37	1.160	65.560	31.315	1.00 24.67	В
ATOM	695	CB	ILE B	37	0.429	64.223	31.230	1.00 24.72	В
ATOM	696	CG2	ILE B	37	-1.085	64.410	31.416	1.00 29.15	В
MOTA	697	CG1	ILE B	37	0.700	63.581	29.879	1.00 22.40	В
ATOM	698	CD1	ILE B	37	0.023	62.237	29.714	1.00 24.46	B
MOTA	699	C	ILE B	37	0.734	66.295	32.579	1.00 25.86	В
ATOM	700	Ö	ILE B	37	-0.019	67.255	32.517	1.00 25.23	B
ATOM	701	N	LYS B	38	1.242	65.840	33.722	1.00 25.23	B
ATOM			LYS B	38	0.967	66.449	35.020		
ATOM	702 703	CA	LYS B	38	1.656	65.652	36.130	1.00 22.96 1.00 22.07	B B
	703	CB	LYS B	38	0.953	64.410	36.522	1.00 25.14	
ATOM									В
ATOM	705	CD	LYS B	38	-0.225	64.727	37.423	1.00 28.48	В
ATOM	706	CE	LYS B	38	-1.014	63.468	37.617	1.00 28.77	В
ATOM	707	NZ	LYS B	38	-1.331	62.953	36.269	1.00 34.06	В
ATOM	708	C	LYS B	38	1.458	67.877	35.102	1.00 23.87	₿
ATOM	709	0	LYS B	38	0.770	68.736	35.640	1.00 20.93	В
ATOM	710	N	GLN B	39	2.662	68.140	34.593	1.00 26.53	В
MOTA	711	CA	GLN B	39	3.189	69.493	34.682	1.00 30.76	₿

Figure 11L

ATOM	712	CB	GLN	B	39	4.629	69.583	34.197	1.00 33.05	В
ATOM	713	CG	GLN	$\mathbf{E}$	39	5.436	70.614	34.985	1.00 43.49	В
ATOM	714	CD	GLN	В	39	4.822	72.026	35.008	1.00 48.65	В
MOTA	715	OEl	GLN	В	39	4.889	72.774	34.021	1.00 51.46	В
ATOM	716	NES	GLN	3	39	4.220	72.389	36.143	1.00 47.35	В
ATOM	717	C	GLN	B	39	2.343	70.417	33.843	1.00 31.81	В
ATOM	718	0	GLN	В	39	2.125	71.574	34.206	1.00 31.08	В
MOTA	719	N	LEU		40	1.897	69.904	32.703	1.00 31.01	В
ATOM	720	CA	LEU		40	1.065	70.671	31.807	1.00 33.41	В
MOTA	721	CB	LEU		40	0.872	69.886	30.517	1.00 32.63	B
ATOM	722	CG	LEU		40	-0.126	70.405	29.482	1.00 34.65	B
ATOM	723		LEU		40	0.171	71.843	29.092	1.00 35.24	В
ATOM	724	CD2	LEU		40	-0.058	69.495	28.281	1.00 35.90	В
ATOM	725	c	LEU		40	-0.289	70.943	32.469	1.00 36.85	В
MOTA	726	0	LEU		40	-0.874	72.010	32.314	1.00 30.83	B
MOTA	727	N	GLN		41	-0.768	69.964	33.215	1.00 36.13	B
ATOM	728	CA	GLN		41	-2.046	70.063	33.894	1.00 30.13	B
ATOM	729	CB	GLN		41	-2.369	68.718	34.517	1.00 41.31	B
ATOM	730	CG	GLN		41	-3.833	68.459	34.735	1.00 47.08	B
ATOM	731	CD	GLN		41	-4.070	67.139	35.420	1.00 54.09	В
ATOM	732	OE1	GLN		41	-3.517	66.102	35.013	1.00 55.42	B
ATOM	733	NE2	GLN		41	-4.908	67.154	36.461	1.00 54.90	B
ATOM	734	C	GLN		41	-2.039	71.148	34.974	1.00 39.95	B
ATOM	735	ō	GLN		41	-2.988	71.925	35.089	1.00 39.23	B
ATOM	736	N	ALA		42	-0.972	71.194	35.767	1.00 39.05	B
ATOM	737	CA	ALA		42	-0.845	72.188	36.824	1.00 38.56	B
ATOM	738	CB	ALA		42	0.345	71.852	37.757	1.00 34.14	B
MOTA	739	c	ALA		42	-0.647	73.566	36.228	1.00 40.18	B
ATOM	740	ō	ALA		42	~1.139	74.560	36.765	1.00 41.44	B
ATOM	741	N	ARG		43	0.078	73.634	35.118	1.00 41.44	а В
ATOM	742	CA	ARG		43	0.340	74.910	34.476	1.00 43.71	B
ATOM	743	CB	ARG		43	1.242	74.713	33.260	1.00 47.26	В
ATOM	744	CG	ARG		43	1.703	75.997	32.592	1.00 51.08	B
ATOM	745	CD	ARG		43	2.582	75.677	31.401	1.00 54.95	B
ATOM	746	NE	ARG		43	3.778	74.947	31.813	1.00 57.04	В
ATOM	747	CZ	ARG		43	4.819	75.499	32.428	1.00 56,95	B
ATOM	748		ARG		43	4.816	76.794	32.703	1.00 55.89	B
ATOM	749		ARG		43	5.858	74.753	32.781	1.00 57.00	В
ATOM	750	C	ARG		43	-0.987	75.521	34.048	1.00 42.38	B
MOTA	751	Õ		В	43	-1.308	76.657	34.398	1.00 41.41	B
ATOM	752	N	ILE		44	-1.756	74.736	33.310	1.00 41.63	B
ATOM	753	CA	ILE		44	-3.059	75.143	32.810	1.00 43.24	В
ATOM	754	CB		В	44	-3.634	74.085	31.866	1.00 44.23	В
ATOM	755	CG2		В	44	~5.083	74.403	31.592	1.00 45.04	B
ATOM	756	CG1		В	44	-2.778	73.964	30.600	1.00 47.45	В
ATOM	757	CD1		3	44	-3.156	72.745	29.719	1.00 49.42	В
ATOM	758	C		В	44	-4.081	75.306	33.935	1.00 42.37	В
ATOM	759	Ö		В	44	-4.422	76.416	34.332	1.00 42.08	8
ATOM	760	N		В	45	-4.573	74.162	34.398	1.00 42.20	В
ATOM	761	CA	LEU		45	-5.564	74.042	35.450	1.00 43.16	B
ATOM	762	СВ	LEU		45	-6.041	72.592		1.00 46.08	B
MOTA	763	CG	LEU		45	-6.459	72.001	34.162	1.00 47.45	3
MOTA	764		LEU		45	-7.011	70.594	34.357	1.00 47.51	В
ATOM	765		LEU		45	-7.504	72.899	33.521	1.00 48.61	В
ATOM	766	C	LEU		45	-5.016	74.467	36.810	1.00 42.48	B
ATOM	767	ō	LEU		45	-5.674	75.260	37.483	1.00 45.15	В
ATOM	768	NT	LEU		45	-3.945	73.987	37.206	1.00 45.66	3
ATOM	769	CA	ACE		0	15.143	11.286	26.819	1.00 82.49	C
MOTA	770	C	ACE		Ö	14.856	12.476	27.674	1.00 82.44	C
ATOM	771	ō	ACE		0	13.700	12.858	27.851	1.00 84.06	c
	_	-		-	-			· · ·		_

Figure 11M

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

Inventors:

Debra M. Eckert, et al.

ATOM	772	N	ARG	С	1	15.890	13.103	28.220	1.00 82.91	C
ATOM	773	CA	ARG	С	1	15.663	14.253	29.073	1.00 83.87	С
ATOM	774	CB	ARG	Ç	1	16.156	13.970	30.491	1.00 83.74	C
ATOM	775	CG	ARG	C	1	15.769	15.065	31.456	1.00 83.47	C
ATOM	776	CD	ARG	C	1	14.340	15.542	31.156	1.00 81.66	C
ATOM	777	NE	ARG	С	1	13.249	14.748	31.726	1.00 81.00	С
MOTA	778	CZ	ARG	$\mathbb{C}$	1	13.069	13.434	31.597	1.00 79.16	С
ATOM	779	NHl	ARG	С	1	13.901	12.678	30.889	1.00 79.80	С
MOTA	780	NH2	ARG	Ç	1.	12.010	12.875	32.168	1.00 79.18	С
ATOM	781	C	ARG	С	1	16.282	15,541	28.550	1.00 85.03	C
ATOM	782	0	ARG	С	1	15.975	16.644	29.016	1.00 85.10	C
ATOM	783	N	MET	С	2	17.169	15.394	27.581	1.00 85.40	C
ATOM	784	CA	MET	С	2	17.778	16.568	27.012	1.00 86.91	C
ATOM	785	CB	MET	C	2	19.063	16.215	26.290	1.00 88.20	C
MOTA	786	CG	MET	C	2	19.711	17.410	25.653	1.00 89.72	C
ATOM	787	SD	MET	С	2	21.192	16.917	24.823	1.00 94.98	C
ATOM	788	CE	MET	С	2	22.111	16.349	26.176	1.00 91.53	C
ATOM	789	C	MET	C	2	16.771	17.154	26.036	1.00 87.44	С
MOTA	790	0	MET	С	2	16.699	18.368	25.872	1.00 89.05	С
MOTA	791	N	LYS	С	3	16.001	16.278	25.391	1.00 85.66	C
MOTA	792	CA	LYS		3	14.973	16.712	24.444	1.00 83.09	C
ATOM	793	CB	LYS		3	14.033	15.551	24.107	1.00 82.50	C
MOTA	794	CG	LYS		3	12.921	15.895	23.122	1.00 81.54	C
ATOM	795	CD	LYS		3	11.926	14.746	23.005	1.00 81.93	C
ATOM	796	CE	LYS		3	10.866	15.022	21.952	1.00 80.79	C
ATOM	797	NZ	LYS		3	10.154	16.300	22.214	1.00 82.56	С
ATOM	798	С	LYS		3	14.177	17.809	25.128	1.00 82.12	C
ATOM	799	0	LYS		3	14.053	18.925	24.617	1.00 81.76	C
ATOM	800	N	GLN		4	13.651	17.474	26.302	1.00 80.32	C
ATOM	801	CA	GLN		4	12.856	18.401	27.094	1.00 78.87	C
ATOM ATOM	802	CB	GLN		4	12.504	17.759	28.440	1.00 79.91	С
ATOM	803 804	CD	GLN GLN		4 4	12.122 11.087	16.275 15.971	28.356	1.00 80.66	C
ATOM	805		GLN		4	11.348	16.140	27.280 26.082	1.00 81.02 1.00 79.52	C
ATOM	806	NES	GLN		4	9.907	15.516	27.701	1.00 79.52	0
ATOM	807	C	GLN		4	13.667	19.680	27.701	1.00 77.97	C
ATOM	808	0	GLN		4	13.186	20.781	27.032	1.00 78.45	C
ATOM	809	N	ILE		5	14.902	19.530	27.772	1.00 76.07	C
ATOM	810	CA	ILE		5	15.785	20.670	27.974	1.00 73.89	Č
MOTA	811	CB	ILE		5	17.206	20.220	28.381	1.00 73.07	Ċ
ATOM	812		ILE		5	18.175	21.388	28.264	1.00 71.17	Ċ
ATOM	813	CG1	ILE		5	17.174	19.623	29.795	1.00 72.84	č
ATOM	814	CD1	ILE		5	18.518	19.113	30.285	1.00 71.39	Ċ
ATOM	815	C	ILE		5	15.880	21.423	26.656	1.00 74.14	Ċ
ATOM	816	0	ILE	С	5	15.939	22.651	26.628	1.00 73.70	Ċ
MOTA	317	N	GLU	C	6	15.895	20.664	25.567	1.00 73.88	С
ATOM	818	CA	GLU	С	6	15.972	21.222	24.225	1.00 73.70	C
ATOM	819	CB	GLU	С	6	16.395	20.135	23.229	1.00 72.24	C
ATOM	820	CG	GLU	C	6	17.787	19.535	23.464	1.00 69.96	С
ATOM	821	CD	GLU	С	6	18.922	20.428	22.985	1.00 68.01	С
ATOM	822	OE1	GLU	С	6	19.044	21.575	23.461	1.00 65.93	С
MOTA	823	OE2	GLU		6	19.702	19.963	22.125	1.00 68.18	C
MOTA	824	C	GLU		6	14.602		23.842	1.00 74.50	C
MOTA	825	0	GLU		б	14.476	22.546	22.890	1.00 75.27	C
ATOM	826	N	ASP		7	13.577	21.372	24.587	1.00 74.82	C
MOTA	827	CA	ASP		7	12,218	21.838	24.327	1.00 76.17	С
ATOM	828	CB	ASP		7	11.195	20.742	24.644	1.00 77.40	С
ATOM	829	CG	ASP		7	11.408	19.488	23.818	1.00 78.45	С
MOTA	330		ASP		7	11 518	19.609	22.580	1.00 79.26	С
ATOM	831	OD2	ASP	C	7	11.452	18,380	24 404	1.00 79.10	C

Figure 11N

ATOM	832	С	ASP	_	7	11.906	23.079	25,160	1.00 75.92	С
ATOM	833	Ô			7	11.379	24.063	24.643	1.00 75.32	C
ATOM	834	N	LYS		8	12.223	23.024	26.452	1.00 74.05	Ċ
ATOM	835	CA	LYS		8	11.987	24.157	27.336	1.00 71.19	C
ATOM	836	CB	LYS	C	8	12.565	23.886	28.727	1.00 71.19	0
ATOM	837	CG	LYS	C	8	11.647	24.225	29.901	1.00 72.89	
ATOM					8					C
	838	CD	LYS			10.428	23.312	29.921	1.00 75.00	C
ATOM	839	CE	LYS		8	9.587	23.471	31.197	1.00 76.69	C
ATOM	840	NZ	LYS		8	8.998	24.829	31.389	1.00 73.68	c
MOTA	841	C	LYS		8	12.727	25.319	26.679	1.00 69.24	С
ATOM	842	0	LYS	Ç	8	12.295	26.469	26.745	1.00 69.77	C
ATOM	843	N	ILE		9	13.855	25.013	26.046	1.00 65.63	С
ATOM	844	CA	ILE		9	14.609	26.053	25.362	1.00 64.27	С
ATOM	845	CB	ILE		9	15.950	25.511	24.812	1.00 62.88	C
MOTA	846	CG2	ILE		9	16.585	26.515	23.871	1.00 62.42	C
ATOM	847	CG1	ILE		9	16.900	25.231	25.976	1.00 64.19	C
ATOM	848	CD1	ILE		9	18.244	24.656	25.557	1.00 64.32	С
ATOM	849	С	ILE		9	13.756	26.605	24.223	1,00 63.69	С
ATOM	850	0	ILE		9	13.735	27.816	23.985	1.00 63.21	C
MOTA	851	N	GLU	C	10	13.036	25.712	23.543	1.00 62.89	C
ATOM	852	CA	GLU	С	10	12.163	26.092	22.429	1.00 62.21	C
ATOM	853	CB	GLU	С	10	11.419	24.865	21.886	1.00 63.68	C
ATOM	854	CG	GLU	С	10	10.451	25.180	20.751	1.00 66.12	С
ATOM	855	CD	GLU	C	10	9.688	23.961	20.251	1.00 67.29	C
MOTA	856	OE1	GLU	С	10	8.874	24.125	19.318	1.00 69.26	C
ATOM	857	OE2	GLU	С	10	9.894	22.845	20.780	1.00 68.71	C
MOTA	858	С	GLU	С	10	11.142	27.147	22.831	1.00 60.65	C
ATOM	859	0	GLU	С	10	10.991	28.157	22.147	1.00 60.16	С
MOTA	860	N	GLU	C	11	10.429	26.898	23.927	1.00 60.41	С
ATOM	861	CA	GLU	С	11	9.415	27.826	24.435	1.00 58.98	C
ATOM	862	CB	GLU	С	11	8.736	27.243	25.683	1.00 59.35	C
MOTA	863	CG	GLU	C	11	9.709	26.588	26.652	1.00 61.78	C
ATOM	864	CD	GLU	C	11	9.376	26.801	28.127	1.00 63.00	C
ATOM	865	OEl	GLU	C	11	9.329	27.972	28.563	1.00 64.82	С
ATOM	866	OE2	GLU	C	11	9.184	25.804	28.855	1.00 60.50	С
ATOM	867	C	GLU	C	11	10.021	29.186	24.772	1.00 58.03	С
ATOM	868	0	GLU	С	11	9.519	30.229	24.351	1.00 59.21	C
ATOM	869	N	ILE	C	12	11.103	29.178	25.532	1.00 56.15	C
MOTA	870	CA	ILE	С	12	11.765	30.415	25.902	1.00 56.41	C
MOTA	871	CB	ILE	C	12	13.043	30.139	26.710	1.00 55,29	С
MCTA	872	CG2	ILE	С	12	13.791	31.448	26.950	1.00 52.26	Ç
ATOM	873	CG1	ILE		12	12.680	29.404	28.008	1.00 55.06	Ċ
ATOM	874	CD1	ILE	С	12	13.858	29.085	28.914	1.00 55.11	С
MOTA	875	С	ILE	С	1.2	12.132	31.239	24.671	1.00 57.76	Ċ
ATOM	876	0	ILE		12	11.944	32.454	24.659	1.00 59.18	Ċ
ATOM	877	N	GLU		23	12.668	30.589	23.642	1.00 60.62	С
ATOM	878	CA	GLU		13	13.039	31.312	22.423	1.00 62.64	Č
ATOM	879	CB	GLU		13	13.916	30.449	21.497	1.00 66.02	Ċ
ATOM	880	CG	GLU		13	13.319	29.091	21,138	1.00 70.85	Ċ
ATOM	881		GLU		13	14.091	28.355	20.041	1.00 73.58	Ċ
MOTA	882		GLU		13	15.330	28.233	20.163	1.00 72.99	Ċ
ATOM	883		GLU		13	13.456	27.887	19.064	1.00 73.78	Č
ATOM	884	С	GLU		13	11.785	31.748	21.679	1.00 60.74	Ċ
ATOM	885	0	GLU		13	11.808	32.733	20.946	1.00 61 13	C
ATOM	886	N	SER		14	10.695	31.010	21.864	1.00 59.71	C
ATOM	887	CA	SER		14	9.432	31.350	21.211	1.00 60.53	Ċ
ATOM	888	CB	SER		14	8.392	30.248	21.439	1.00 59.88	C
MOTA	889	OG	SER		14	7.157	30.571	20.820	1.00 56.34	c
ATOM	890	C	SER		14	8.921	32.568	21.790	1.00 61.04	c
ATOM	891	0	SER		14	8.793	33.655	21.073	1.00 59.08	C
- A O	بقدائر ب	_	المندب	~	~ <del>~</del>	در، ن	J J - U J J	0 / -	#.UU JJ.UU	_

Figure 110

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, *et al.* 

ATOM	892	N	LYS C	15		8.632	32.671	23.091	1.00	62.79	С
ATOM	893	CA	LYS C	15		8.153	33.873	23.771	1.00	64.30	С
ATOM	894	CB	LYS C	15		7.949	33.612	25.273	1.00	65,74	С
ATOM	895	CG	LYS C	15		6.637	32.903	25.642	1.00	68.25	C
ATOM	896	CD	LYS C	15		6.534	32.695	27.154		69.92	С
ATOM	897	CE	LYS C	15		5.186	32.131	27.564		70.69	Č
ATOM	898	NZ	LYS C	15		4.078	33.079	27.241		73.69	Č
ATOM	899	C	LYS C	15		9.130	35.029	23.601		64.03	Ċ
ATOM	900	Ô	LYS C	15		8.723	36.175	23.408		64.04	Č
MOTA	901	N	GLN C	16		0.418	34.721	23.678		63.47	C
MOTA	902	CA	GLN C	16		1.451	35.733	23.537		65.82	C
				16			35.064	23.393		65.17	
ATOM	903	CB	GLN C			2.813					C
ATOM	904	CG	GLN C	16		3.970 4.944	36.027	23.413		65.29	C
ATOM	905	CD	GLN C	16			35.695	24.516		66.93	
MOTA	906		GLN C	16		5.940	36.389	24.719		68.97	C
ATOM	907	NE2		16		4.657	34.621	25.244		66.55	C
MOTA	908	С	GLN C	16		1.157	36.605	22.317		67.53	С
MOTA	909	0	GLN C	16		1.172	37.836	22.397		68.90	C
ATOM	910	N	LYS C	17		0.886	35.952	21.193		67.63	C
ATOM	911	CA	LYS C	17		0.566	36.648	19.954	1.00		C
ATOM	912	CB	LYS C	17	1	0.355	35.627	18.833	1.00	69.39	C
MOTA	913	CG	LYS C	17		9.747	36.199	17.556	1.00	72.05	С
ATOM	914	CD	LYS C	17	1	0.657	37.203	16.835	1.00	73.47	C
MOTA	915	CE	LYS C	17		9.946	37.784	15.613	1.00	74.71	С
ATOM	916	NZ	LYS C	17	1	0.885	38.603	14.795	1.00	76.15	С
ATOM	917	С	LYS C	17		9.306	37.492	20.123	1.00	66.64	С
ATOM	918	0	LYS C	17		9.244	38.632	19.652	1.00	67.45	С
ATOM	919	N	LYS C	18		300	36.924	20.784	1.00	64.29	С
ATOM	920	CA	LYS C	18		7.049	37.641	21.019		63.62	С
ATOM	921	CB	LYS C	18		5.979	36.719	21.627		64.15	С
ATOM	922	CG	LYS C	18		5.088	36.062	20.586	1.00	66.52	С
ATOM	923	CD	LYS C	18		3.935	35.297	21.220		68.98	Č
ATOM	924	CE	LYS C	18		4.427	34.076	21.970		70.96	Ċ
ATOM	925	NZ	LYS C	18		5.098	33.116	21.040		72.62	Č
ATOM	926	C	LYS C	18		7.265	38.852	21.922		61.00	Ċ
ATOM	927	0	LYS C	18		5.854	39.958	21.585		61.84	Ċ
ATOM	928	N	ILE C	19		7.904	38.653	23.067		56.58	Ċ
ATOM	929	CA	ILE C	19		3.179	39.765	23.961		53.92	C
ATOM	930	CB	ILE C	19		9.101	39.329	25.119		52.10	c
ATOM	931	CG2	ILE C	19		9.719	40.545	25.799		51.95	Ċ
	932	CG1	ILE C	19		3.304	38.463	26.095		51.65	C
MOTA		CD1		19		9.103		27.247		50.93	c
ATOM	933		ILE C	19		3.833	37.908 40.893	23.165		53.24	c
ATOM	934	C									
ATOM	935	0	ILE C	19		3.604	42.069	23.438		52.35	С
ATOM	936	N	GLU C	20		9.642	40.534	22.173		53.82	С
ATOM	937	CA	GLU C	20		294	41.536	21.338		54.86	C
ATOM	938	CB	GLU C	20		1.393	40.910	20.472		55.74	C
ATOM	939	CG	GLU C	20		2.554	40.318	21.251		56.50	C
MOTA	940	CD	GLU C	20		3.683	39.851	20.352		56.98	C
ATOM	941		GLU C	20			38.918			56.87	С
MOTA	942		GLU C	20		1.786	40.427	20.453		58.79	С
ATOM	943	С	GLU C	20		245	42.188	20.437		55.80	С
ATOM	944	0	GLU C	20		3.311	43.382	20.166		55.44	C
MOTA	945	N	ASN C	21		3.289	41.389	19.972		55.46	C
ATOM	946	CA	ASN C	21		7.223	41.899	19.118		57.62	С
ATOM	947	CB	ASN C	21		5.392	40.754	18.530		59.92	С
ATOM	948	CG	ASN C	21	•	7.060	40.101	17.325		63.29	С
MOTA	949	0D1	ASN C	21	6	5.574	39.092	16.806	1.00	62.67	C
MOTA	950	ND2	ASN C	21	8	3.169	40.684	16.856	1.00	61.87	C
MOTA	951	C	ASN C	21	•	5.307	42.829	19.891	1.00	58.25	С

Figure 11P

ATOM	952	0	ASN C	21	5.649	43.697	19.309	1.00 59.75	С
MOTA	953	N	GLU C		6.255		21.206	1.00 56.32	C
ATOM	954	CA	GLU C		5.411		22.030	1.00 53.64	Č
MOTA	955	CB	GLU C		5.014		23.313	1.00 55.42	Ċ
ATOM	956	CG	GLU C		3.786		23.967	1 00 60.12	Č
ATOM	957	CD	GLU C		2.506		23.188	1.00 61.82	Ü
ATOM	958	OE1			2.559		21.942	1.00 62.49	Ċ
ATOM	959	OE2			1.435		23.825	1.00 63.39	C
ATOM	960	C	GLU C		6.158		22.344	1.00 50.89	C
ATOM	961	Õ	GLU C		5.573	45.873	22.282	1.00 49.72	Ċ
ATOM	962	N	ILE C		7.448	44.691	22.665	1.00 47.08	C
ATOM	963	CA	ILE C		8.259		22.948	1.00 46.40	C
ATOM	964	CB	ILE C		9.752	45.504	23.290	1.00 47.53	c
ATOM	965	CG2			10.707	46.653	22.910	1.00 44.86	C
ATOM	966	CG1			9.898		24.783	1.00 45.28	0
ATOM	967	CD1			9.101	44.004	25.256	1.00 45.28	Ċ
ATOM	968	C	ILE C		8.222	46.771	21.717	1.00 46.76	C
ATOM	969	ō	ILE C		8.317	47.999	21.822	1.00 46.87	0
ATOM	970	N	ALA C		8.071	46.137	20.556	1.00 47.50	Ċ
ATOM	971	CA	ALA C		8.002	46.828	19.271	1.00 46.10	C
ATOM	972	CB	ALA C		8.112	45.809	18.126	1.00 44.51	C
ATOM	973	c	ALA C		6.706	47 644	19.137	1.00 45.09	C
ATOM	974	Ö	ALA C		6.741	48.810	18.752	1.00 43.05	C
ATOM	975	N	ARG C		5.566	47.034	19.445	1.00 43.64	C
ATOM	976	CA	ARG C		4.301	47.753	19.346	1.00 45.79	C
ATOM	977	CB	ARG C		3.115	46.807	19.581	1.00 44.07	c
ATOM	978	CG	ARG C		3.045	45.680	18.564	1.00 48.16	0
ATOM	979	CD	ARG C		1.677	44.986	18.458	1.00 48.18	c
MOTA	980	NE	ARG C		1.216	44.299	19.664	1.00 54.12	C
ATOM	981	CZ	ARG C		0.665	44.888	20.725	1.00 58.36	C
ATOM	982		ARG C		0.475	46.206	20.756	1.00 59.26	C
ATOM	983		ARG C	25	0.268	44.148	21.755	1.00 59.83	C
ATOM	984	C	ARG C	25	4.257	48.908	20.345	1.00 47.24	Ċ
ATOM	985	ō	ARG C	25	3.941	50.038	19.978	1.00 50.68	c
ATOM	986	N	ILE C	26	4.584	48.617	21.601	1.00 47.54	Ċ
ATOM	987	CA	ILE C	26	4.591	49.608	22.673	1.00 44.40	č
ATOM	988	CB	ILE C	26	5.042	48.959	24.001	1.00 43.91	C
ATOM	989	CG2	ILE C	26	5.259	50.026	25.071	1.00 45.47	C
ATOM	990	CG1	ILE C	26	4.010	47.930	24.450	1.00 42.59	C
ATOM	991	CD1	ILE C	26	4.445	47.138	25.663	1.00 40.19	č
ATOM	992	С	ILE C	26	5.532	50.766	22.379	1.00 44.58	č
ATOM	993	Ō	ILE C	26	5.193	51.935	22.564	1.00 42.04	č
ATOM	994	N	LYS C	27	6.721	50.422	21.919	1.00 46.75	Č
ATOM	995	CA	LYS C	27	7.754	51.394	21.619	1.00 51.78	č
ATOM	996	CB	LYS C	27	8.915	50.674	20.951	1.00 54.23	Ċ
ATOM	997	CG	LYS C	27	10.184	51.465	20.863	1.00 57.21	C
ATOM	998	$\mathbb{C}\mathbb{D}$	LYS C	27	11.313	50.479	20.644	1.00 60.99	C
ATOM	999	CE	LYS C	27	12.660	51.064	21.014	1.00 62.83	C
MOTA	1000	NZ	LYS C	27	13.750	50.060	20.828	1.00 64.49	Ċ
ATOM	1001	C	LYS C	27	7.299	52.556	20.750	1.00 52,44	Ċ
ATOM	1002	O	LYS C	27	7.334	53.710	21.165	1.00 54.11	С
MOTA	1003	N	LYS C	28	6.877	52.239	19.538	1.00 53.88	С
MOTA	1004	CA	LYS C	28	6.435	53.250	18.599	1.00 55.29	C
MOTA	1005	СЭ	LYS C	28	6.169	52.582	17.249	1.00 57.59	Ĉ
MOTA	1006	CG	LYS C	28	7.390	51.841	16.717	1.00 59.15	C
ATOM	1007	CD	LYS C	28	7.041	50.830	15.635	1.00 62.19	С
ATOM	1008	CE	LYS C	28	8.292	50.088	15.158	1.00 63.12	C
MOTA	1009	NZ	LYS C	28	9.029	49.411	16.282	1.00 65.69	С
MCTA	1010	C	LYS C	28	5.187	53.931	19.122	1.00 55.14	С
MOTA	1011	0	LYS C	28	5.052	55.147	19.030	1.00 57.43	C

Figure 11Q

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM	1012	N	LEU C	29	4,275	53.138	19.671	1.00 52.27	С
MCTA	1013	CA	LEU C	29	3.025	53.649	20.214	1.00 51.04	Ċ
MOTA	1014	CB	LEU C	29	2.281	52.485	20.855	1.00 51.13	C
MOTA	1015	CG	LEU C	29	0.776	52.493	21,051	1.00 50.66	С
ATOM	1016	CD1	LEU C	29	0.051	52.868	19.755	1.00 51.59	Ċ
ATOM	1017	CD2	LEU C	29	0.389	51.100	21,491	1.00 50.29	č
ATOM	1018	C	LEU C	29	3.347	54.739	21.245	1.00 50.83	č
ATOM	1019	ō	LEU C	29	2.739	55.805	21.269	1.00 53.58	č
ATOM	1020	N	LEU C	30	4.327	54.457	22.089	1.00 50.52	Ċ
MOTA	1021	CA	LEU C	30	4.767	55.397	23.100	1.00 48.88	Ċ
ATOM	1022	CB	LEU C	30	5.813	54.730	23.997	1.00 48.03	Ĉ
ATOM	1023	CG	LEU C	30	6.485	55.530	25.113	1.00 47.31	Č
MOTA	1024	CD1	LEU C	30	5.447	56.172	26.033	1.00 45.24	C
ATOM	1025	CD2	LEU C	30	7.398	54.575	25.889	1.00 48.28	č
ATOM	1026	C	LEU C	30	5.374	56.587	22.379	1.00 48.83	C
ATOM	1027	0	LEU C	30	5.020	57.736	22.642	1.00 48.40	c
	1027		GLN C	31	6.298	56.289	21.470	1.00 49.93	C
ATOM	1029	N CA	GLN C	31	6.983	57.304	20.670	1.00 52.00	C
MOTA MOTA	1030	CB	GLN C	31	7.822	56.609	19.590	1.00 35.56	C
		CG	GLN C	31	8.628	57.513	18.645	1.00 53.56	C
ATOM	1031			31	9.768	58.241	19.333		
MOTA	1032	CD OE1	GLN C	31	10.233	57.818	20.391	1.00 64.58	C
ATOM	1033	NE2						1.00 68.00 1.00 64.37	C
MOTA	1034		GLN C	31	10.249	59.318	18.715		C
ATOM	1035	C	GLN C	31	5.947	58.225		1.00 49.56	C
ATOM	1036	0	GLN C	31	6.192	59.415	19.814	1.00 45.68	C
MOTA	1037	N	LEU C	32	4.793	57.657	19.675 19.034	1.00 47.64	C
ATOM	1038	CA	LEU C	32	3.723	58.401	18.461	1.00 48.95	C
MOTA	1039	CB	LEU C	32	2.689	57.433		1.00 50.72	C
MOTA	1040	CG	LEU C	32	1.602	57.935	17.502	1.00 51.93	C
ATOM	1041	CD1	LEU C	32	2.209 0.554	58.293 56.840	16.154 17.313	1.00 50.26 1.00 51.55	C
MOTA	1042	CD2	LEU C	32					C
ATOM	1043	C		32	3.070	59.295	20.077	1.00 49.32	C
ATOM	1044	0	LEU C	32	3.040	60.519	19.929	1.00 50.01	C
MOTA	1045	N	THR C	33	2.545	58.659	21.125	1.00 48.74	C
ATOM	1046	CA	THR C	33	1.878	59.324	22.246	1.00 43.86	C
ATOM	1047	CB	THR C	33	1.643	58.329	23.400	1.00 46.04	C
ATOM	1048	OG1	THR C	33	0.707	57.332	22.977	1.00 47.18	C
ATOM	1049	CG2	THR C	33	1.121	59.039	24.639	1.00 42.89	C
MOTA	1050	С	THR C	33	2.683	60.494	22.771	1.00 41.04	C
ATOM	1051	0	THR C	33	2.132	61.537	23.122	1.00 39,26	C
ATOM	1052	M	VAL C	34	3.992	60.303	22.843	1.00 38.83	C
MOTA	1053	CA	VAL C	34	4.886	61.346	23.301	1.00 36.90	C
ATOM	1054	CB	VAL C	34	6.329	60.825	23.377	1.00 33.71	C
ATOM	1055	CG1	VAL C	34	7.270	61.907	23.904	1.00 29.40	С
ATOM	1056	CG2	VAL C	34	6.366	59.590	24.251	1.00 31.78	C
ATOM	1057	C	VAL C	34	4.795	62.437	22.254	1.00 38.65	C
ATOM	1058	0	VAL C	34	4.489	63.595	22.556	1.00 39.38	C
ATOM	1059	N	TRP C	35	5.049	62.038	21.010	1.00 42.18	C
MOTA	1060	CA	TRP C	35	5.002	62.937	19.868	1.00 40.00	C
ATOM	1061	CB	TRP C	35	4.991	62.134	18.563	1.00 40.06	C
ATOM	1062	CG	TRP C	35	4.848	63.020	17.399	1.00 36.56	C
MOTA	1063		TRP C	35	3.696	63.161	16.561	1.00 36.91	C
ATOM	1064		TRP C	35	3.968	64.212	15.673	1.00 41.20	C
ATOM	1065	CE3	TRP C	35	2.457	62.505	16.503	1.00 40.31	C
MOTA	1066		TRP C	35	5.748	63.944	16.974	1.00 35.30	C
ATOM	1067	NE1	TRP C	35	5.228	64.673	15.945	1.00 39.45	C
MOTA	1068		TRP C	35	3.037	64.643	14.704	1.00 38.75	C
ATOM	1059	CZ3		35	1.528	62.934	15.541	1.00 39.54	C
ATOM	1070	CH2		35	1.827	63.984	14.651	1.00 41.30	C
ATOM	1071	С	TRP C	35	3.764	63.833	19.901	1 00 39.80	С

Figure 11R

ATOM	1072	0	TRP C	35	3.868	65.052	19.769	1.00 38,39	С
ATOM	1073	N	GLY C	36	2.601	63.210	20.059	1.00 36.88	Ċ
ATOM	1074	CA	GLY C	36	1.356	63.957	20.103	1.00 38.94	č
MOTA	1075	C	GLY C	36	1.315	64.973	21.226	1.00 38.45	č
	1076			36	0.931			1.00 37.76	
ATOM		0	GTA C			66.114	21.001		C
MOTA	1077	N	ILE C	37	1.700	64.557	22.435	1.00 40.86	С
ATOM	1078	CA	ILE C	37	1.724	65.442	23.604	1.00 36.66	С
ATOM	1079	CB	ILE C	37	2.352	64.755	24.857	1.00 36.83	С
MOTA	1080	CG2	ILE C	37	2.489	65.766	26.005	1.00 27.32	C
ATOM	1081	CGl	ILE C	37	1.512	63.548	25.275	1.00 37.14	C
ATOM	1082	CD1	ILE C	37	2.066	62.794	26.501	1.00 35.85	С
ATOM	1083	С	ILE C	37	2.587	66.655	23.284	1.00 38.37	Ç
ATOM	1084	ō	ILE C	37	2.187	67.788	23.529	1.00 37,68	č
ATOM	1085	N	LYS C	38	3.775	66.399	22.740	1.00 40.28	ć
				38	4.717	67.456	22.381	1.00 40.28	C
MOTA	1086	CA	LYS C						
MOTA	1087	CB	LYS C	38	5.927	66.868	21.639	1.00 46.36	C
ATOM	1088	CG	LYS C	38	7.109	67.829	21.391	1.00 52.00	C
ATOM	1089	CD	LYS C	38	8,125	67.162	20.433	1.00 56.10	С
ATOM	1090	CE	TAZ C	38	9.365	68.008	20.096	1.00 56.61	С
ATOM	1091	NZ	LYS C	38	10.340	68.155	21.222	1.00 59.57	Ç
ATOM	1092	C	LYS C	38	3.995	68.445	21.483	1.00 42.06	C
ATOM	1093	0	LYS C	38	4.351	69.628	21.428	1.00 41.76	C
ATOM	1094	N	GLN C	39	2.977	67.966	20.774	1.00 39.73	C
MOTA	1095	CA	GLN C	39	2,232	68.862	19.908	1.00 40.05	C
ATOM	1096	CB	GLN C	39	1.499	68.100	18.778	1.00 41.27	Ċ
ATOM	1097	CG	GLN C	39	2.385	67.148	17.928	1.00 42.44	Č
				39	3.681				C
MOTA	1098	CD	GLN C			67.786	17.465	1.00 42.00	
ATOM	1099	OE1		39	3.678	68.822	16.813	1.00 44.81	C
ATOM	1100	NE2		39	4.802	67.163	17.802	1.00 46.04	C
ATOM	1101	С	GLN C	39	1.241	69.638	20.781	1.00 36.22	C
ATOM	1102	0	GLN C	39	1.344	70.845	20.885	1.00 34.78	C
ATOM	1103	N	TER C	40	0.285	68.950	21.398	1.00 34.58	C
MOTA	1104	CA	LEU C	40	-0.696	69.625	22.268	1.00 36.22	C
ATOM	1105	CB	LEU C	40	-1.465	68.595	23.096	1.00 34.67	С
ATOM	1106	CG	LEU C	40	-2.365	69.192	24.186	1.00 34.61	C
MOTA	1107	CD1	LEU C	40	-3.392	70.142	23.510	1.00 34.28	С
ATOM	1108	CD2	LEU C	40	-3.057	68.084	24.972	1,00 30,45	C
ATOM	1109	С	LEU C	40	-0.029	70.630	23.226	1.00 36.51	Č
ATOM	1110	Ö	LEU C	40	-0.494	71.755	23.419	1.00 36.17	Ċ
ATOM	1111	N	GLN C	41	1.068	70.220	23.832	1.00 36.56	Ċ
				41	1.764	71.106	24.751	1.00 38.77	C
ATOM	1112	CA	GLN C						
MOTA	1113	CB	GLN C	41	2.883	70.310	25.433	1.00 38.66	C
ATOM	1114	CG	GLN C	41	3.606	70.994	26.582	1.00 46.41	C
ATOM	1115	CD	GLN C	41	4.245	69.979	27.529	1.00 50.25	C
MOTA	1116	OEI	GLN C	41	4.898	69.028	27.091	1.00 53.94	C
ATOM	1117	NE2	GLN C	41	4.063	70.180	28.831	1.00 52.04	C
ATOM	1118	С	GLN C	41	2.291	72.336	23.998	1.00 37.58	C
MOTA	1119	0	GLN C	41	2.190	73.466	24.486	1.00 38.73	C
ATOM	1120	N	ALA C	42	2.827	72.128	22.795	1.00 36.75	C
ATOM	1121	CA	ALA C	42	3.365	73.249	22.014	1.00 36.93	С
ATOM	1122	CB	ALA C	42	4.084	72.717	20.779	1.00 32.48	C
ATOM	1123	C	ALA C	42	2.241	74.209	21.500	1.00 35.85	Ċ
ATOM	1123	0	ALA C	42	2.407	75.427	21.602	1.00 34.18	ç
					1.101		21.249	1.00 32.51	č
ATOM	1125	N	ARG C	43		73.629			C
MOTA	1126	CA	ARG C	43	-0.072	74.365	20.829	1.00 34.59	
ATOM	1127	CB	ARG C	43	-1.152	73.357	20.524	1.00 34.80	C
ATOM	1128	CG	ARG C	43	-2.467	73.891	20.060	1.00 36.54	C
MOTA	1129	CD	ARG C	43	-3.310	72.667	19.769	1.00 37.93	C
ATOM	1130	NE	ARG C	43	-4.631	72.945	19.236	1.00 40.51	С
ATOM	1131	CZ	ARG C	43	-5.491	71.985	18,901	1.00 42.74	С

Figure 11S

Docket/App No.: 0399.1192-008
Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

ATOM	1132	NH1	. AR	3 C	4.3	_	-5.127	70.717	19.051	1.00 41.4	0 с
ATOM	1133	NHI	AR	G C	43		-6.676				_
ATOM	1134	C	ARG	3 C	43		-0.568				-
ATOM	1135	0		G C			1.049				_
MOTA	1136	N		E C			-0.434			1.00 41.6	
MOTA	1137	CA	ILI	E C	44		-0.901				
ATOM	1138	CB	IL		44		1.403				
ATOM	1139	CG2			44		1.802			1.00 46.23	_
ATOM	1140	CG1			44		2.572				
ATOM	1141	CD1			44		2.926			1.00 50.33	
ATOM	1142	C	ILE		44		0.109			1.00 41.15	
ATOM	1143	0	ILE		44		0.235			1.00 40.03	_
MOTA	1144	N	LEU		45		1.345			1.00 40.33	_
ATOM	1145	CA	LEU		45		2.401			1.00 39.81	
ATOM	1146	CB	LEU		4.5		3.357			1.00 40,22	
ATOM	1147	CG	LEU		45		2.889			1.00 40.80	_
ATOM	1148	CD1			45		1.733		27.364	1.00 42.51	
ATOM	1149	CD2			45		4.029		28.299	1.00 39.44	
ATOM	1150	C	LEU		45		3.215		24.540	1.00 38.95	
ATOM	1151	0	LEU		45		3.071		23.327	1.00 39.83	
ATOM	1152	NT	LEU		4.5		4.014	78.810	24.964	1.00 39.47	
ATOM	1153	OH2			2		8.280		27.138	1.00 38.82	
ATOM	1154	OH2	TIF	W	3		8.782	24.001	17.582	1.00 78.47	
ATOM	1155	OH2	TIF		4		0.492	62.209	33.896	1.00 50.43	
ATOM	1156	OH2	TIP		5		6.020	70.609	23.199	1.00 45.29	
ATOM	1157	OH2	TIP		6		1.993	78.695	31.896	1.00 37.25	
ATOM	1158	OH2	TIP	W	7		0.294	18.975	19.485	1.00 49.56	
ATOM	1159	OH2	TIP	W	8		8.592	15.442	35.405	1.00 34.86	
ATOM	1160	OH2	TIP	W	9		5.907	64.337	32.524	1.00 31.24	W
ATOM	1161	OH2	TIP	W	10		1.567	18.853	30.945	1.00 47.94	W
ATOM	1162	OH2	TIP	W	11	-9	9.321	65.456	23.794	1.00 46.60	W
ATOM	1163	OH2	TIP	W	12	-3	2.842	65.953	28.078	1.00 59.15	W
ATOM	1164	OH2	TIP	W	13	-1	1.409	77.305	18.859	1.00 37.51	W
MOTA	1165	OH2	TIP	W	24		5.597	64.224	37.408	1.00 39.02	W
ATOM	1166	OH2	TIP	W	15	-5	5.079	75.908	18.460	1.00 48.65	W
ATOM	1167	OH2	TIP	W	16	12	2.444	58.431	21.920	1.00 62.97	W
ATOM	1168	OH2	TIP	W	17	-12	2.927	70.555	24.520	1.00 61.81	W
ATOM	1159	OH2	TIP	W	18	14	1.897	23.356	34.046	1.00 40.13	W
ATOM	1170	OH2	TIP	W	19	3	3.154	40.721	28.964	1.00 29.89	W
ATOM	1171	OH2	TIP	W	20	4	1.290	81.951	24.440	1.00 44.83	W
ATOM	1172	OH2	TIP	W	21	26	.490	23.104	32.265	1.00 62.67	W
ATOM	1173	OH2	TIP	W	22	13	.085	59.162	33.622	1.00 54.53	W
ATOM	1174	OH2		W	23		1.166	45.626	35.200	1.00 56.34	W
ATOM	1175	OH2	TIP	W	24		.278	62.692	33.867	1.00 64.05	W
ATOM	1176	OH2	TIP	W	25		.697	10.892	29.710	1.00100.00	W
ATOM	1177	OH2		W	26		.281	39.194	26.136	1.00 62.29	W
ATOM	1178	OH2		W	27		.833	20.843	19.882	1.00 59.57	W
ATOM	1179	OH2	TIP		28		.030	74.838	23.517	1.00 53.18	W
MOTA	1180	OH2	TIP		29		.246	80.456	24.973	1.00 36.18	W
MOTA	1181	OH2			30		.034	76.181	17.506	1.00 50.44	W
ATOM	1182	OH2			31		.424	49.275	18.155	1.00 44.03	W
MOM	1183				32		.269	64.921	23.710	1.00 31.68	W
ATOM	1184	OH2			33		.134	28.497	40.798	1.00 60.31	W
ATOM ATOM	1185	OH2			34		.326	28.221	41.517	1.00 85.52	W
	1186	OH2			35		.492	26.009	31.850	1.00 68.20	W
ATOM	1187		TIP		36		.270	23.540	41.621	1.00 45.61	W
MOTA MOTA	1188	OH2			37		.175	27.169	41.299	1.00 57.26	W
ATOM ATOM	1189	OH2			38		.133	30.154	42.769	1.00 94.65	M
	1190	OH2			39		.961	29.473	38.207	1.00 73.43	W
ATOM	1191	OHO	11 11 11	W	40	26	.646	30.299	35.030	1.00 86.46	M

Figure 11T

ATCM	1192	OH2 T	IP V	V 41	21.799	33.921	37.475	1.00 98.23	W
MOTA	1193	OH2 T	IP V	42	12.296	24.508	37.800		W
MOTA	1194	OH2 T	IP V	43	10.910	28.524	40.599		W
ATOM	1195		IP M	i 44	8.726	30.065	36.214		W
ATOM	1196		IP W	1 45	20.748	34.061	34.804		W
ATOM	1197	OH2 T	IP W	7 45	7.462	29.159	29.170	1.00 88.23	W
ATOM	1198		IP W		7.466	31.280	33.124		W
MOTA	1199		IP W		6.666		36.241		M
ATOM	1200		IP W		3.823	27.148	35.557	1.00 92.76	W
ATOM	1201		IP W		7.608		32.367	1.00 83,54	W
ATOM	1202		IP W		10.064		38,975	1.00 68.12	W
ATOM	1203		IP W		14.649		38.236	1.00 73.09	W
MOTA	1204		IP W		16.799		39.778		M
ATOM ATOM	1205		IP W		15.456		39.598		W
ATOM	1206 1207		IP W		8.442	41.891	37.753	1.00 57.63	W
ATOM	1208		IP W		9.926	44.040	39.986	1.00 80.20	M
ATOM	1209		IP W		3.713	35.630	32.034	1.00 65.94	W
ATOM	1210		IP W IP W		4.004	32.569	30.481	1.00 98.02	W
ATOM	1211		IP W	59 40	13.514	45.594	36.374	1.00 45.92	W
ATOM	1212		IP W	60 61	12.274	44.358	32.693	1.00 69.72	W
ATOM	1213		IP W	62	-1.770 -0.747	41.459	30.288	1.00 86.62	W
ATOM	1214		IP W	63		39.619	34.003	1.00 85.57	W
ATOM	1215		IP W	64	2.370 7.646	42.056 47.813	36.997	1.00 63.26	M
ATOM	1216		P W	65	-1.942	50.096	26.559	1.00 86.77	W
ATOM	1217		PW	66	-0.455	48.262	25.818	1.00 33.47	W
ATOM	1218		PW	67	-1.850	44.976	24.057 32.352	1.00 48.49	W
ATOM	1219		PW	68	-4.779	47.469	30.587	1.00 46.88 1.00 53.38	W
MCTA	1220		PW	69	-8.800	47.417	33.155	1.00 53.38 1.00 55.34	W
ATOM	1221		P W	70	-7.762	51.374	35.608	1.00 35.34	W
ATOM	1222	OH2 TI	P W	71	5.493	50.307	35.418	1.00 63.93	W tar
ATOM	1223	OH2 TI	PW	72	-2.293	60.557	33.176	1.00 58.13	W
MOTA	1224	OH2 TI	PW	73	-3.891	59.956	22.859	1.00 42.99	W
MOTA	1225	OH2 TI	P W	74	-2.324	52.365	23.808	1.00 68.12	W
ATOM	1226	OH2 TI	P W	75	-4.610	53.603	23.534	1.00 99.86	W
ATOM	1227	OH2 TI	P W	76	-5.369	51.351	24.806	1.00 66.59	W
ATOM	1228	OH2 TI	P W	77	-9.158	53.927	27.711	1.00 59.38	W
MOTA	1229	OH2 TI	РW	78	-6.839	60.379	22.155	1.00 48.43	W
MOTA	1230	OH2 TI		79	-7.811	55.209	31.835	1.00 63.25	W
ATOM	1231		P W	80	-8.988	55.740	34.680	1.00 48.03	W
ATOM	1232	OH2 TI		81	-14.358	62.793	31.478	1.00 77.34	W
ATOM	1233		ΡW	82	-14.884	67.194	30.264	1.00100.00	W
ATOM	1234	OH2 TI		83	-13.964	62.903	27.850	1.00 61.59	W
ATOM	1235	OH2 TI		84	-16.467	64.338	27.598	1.00 62.99	W
ATOM	1236	OH2 TI		85	-14.165	71.419	31.235	1.00 58.55	W
ATOM ATOM	1237	OH2 TI		86	-12.150	75.052	20.683	1.00 54.74	W
ATOM	1238 1239	OH2 TI		87	-15.348	66.527	23.972	1.00 86.65	W
ATOM	1240	OH2 TI		88	23.657	18.784	16.110	1.00 46.11	W
				89	21.774	13.448	17.383	1.00 55.62	W
ATOM ATOM	1241 1242	OH2 TI		90	28.955	20.801	18.398	1.00 47.29	W
ATOM	1243	OH2 TIE		91	19.043	22.428	18.931	1.00 70.31	W
ATOM	1243	OH2 TIE		92	32.348	21.741	32.055	1.00 80.85	W
ATOM ATOM	1244	OH2 TIE		93 94	31.544	26.386	31.293	1.00 80.53	W
ATOM	1246	OH2 TIP		95	30.484 28.981	31.504	24.099	1.00 51 19	W
ATOM	1247	OH2 TIE		96	25.233	30.812	18.458	1.00 98.45	W
ATOM	1248	OH2 TIP		97	25.740	35.680 37.432	28.569	1.00 53.47	W
ATOM	1249	OH2 TIP		98	18.343		31.266	1.00 96.40	W
ATOM	1250	OH2 TIP		99	26.162	27.853	17.008	1.00 87.39	W
ATOM	1251	OH2 TIP			18.896	37.649	24.887 32.149	1.00 63.29	W
					20.000	J / . U 4 J	22.143	1.00 75.85	W

Figure 11U

MOTA	1250	OH2	TIP	W	101	20.897	31.301	18.264		88.40	W
ATOM	1253	OH2	TIP	W	102	19.191	42.582	21.450		55.18	W
ATOM	1254		TIP			23.958	41.188	26.907		78.30	W
ATOM	1255		TIP			18.433	46.716	22.932	1.00	54.59	W
ATOM	1256		TIP			22.353	48.547	25.042	1.00	59.94	W
ATOM	1257		TIP			21.797	41.049	34.496	1.00	78.60	W
	1258				107	21.437	46.210	33.535	1.00	75.53	W
ATOM			TIP			14.907	43.959	21.380	1.00	54.65	W
ATOM	1259					15.635	42.456	19.119		58.03	W
MOTA	1260		TIP			19.533	44.310	33.666		80.58	W
MOTA	1261				110		50.736	29.399		60.97	W
MOTA	1262		TIP			18.747		28.680		55.70	W
MOTA	1263		TIP			21.131	52.757			72.59	W
MOTA	1264		TIP		113	17.303	55.311	38.133			W
MOTA	1265	OH2	TIP	W	114	18.939	58.215	28.845		79.75	W
ATOM	1266	OH2	TIP	W	115	14.666	59.680	28.964		50.64	
ATOM	1267	OH2	TIP	W	116	17.408	62.649	28.523		74.43	W
ATOM	1268	OH2	TIP	W	117	12.106	61.533	23.810		89.64	W
ATOM	1269	OH2	TIP	W	118	10.138	60.131	37.626		89.60	W
ATOM	1270	OH2	TIP	W	119	14.125	60.999	36.831		78.03	W
MOTA	1271		TIP	W	120	6.987	65.584	27.400	1.00	63.28	W
ATOM	1272	OH2			121	8.699	65.761	30.950	1.00	64.96	W
ATOM	1273	OH2	TIP			11.912	66.582	33.458	1.00	45.24	W
ATOM	1274	OH2	TIP			7.712	69.520	31.053	1.00	89.81	W
ATOM	1275	OHZ			124	0.300	66.328	28.053		83.63	W
	1275	OH2	TIP			18.739	12.093	36.575		68.16	W
ATOM			TIP			8.341	17.901	23.874		69.12	W
ATOM	1277	OH2	TIP			6.665	20.667	30.766		79.31	W
ATOM	1278	OH2				13.178	21.216	32.239		55.97	W
ATOM	1279	OH2	TIP				21.187	21.255		66.56	W
MOTA	1280	OH2	TIP			7.700		19.828		40.17	W
MOTA	1281	OH2	TIP			17.038	26.024	16.376		77.12	W
ATOM	1282	QH2			131	9.682	31.384			59.43	W
ATOM	1283	OH2	TIP			11.568	29.117	15.187			W
MOTA	1284	OH2	TIP			2.602	30.287	27.387		64.52	M
ATOM	1285	OH2			134	10.743	41.812	16.813		84.35	W
MOTA	1286	OH2	TIP	W	135	13.070	38.706	12.664		61.24	
ATOM	1287	OH2	TIP	W	136	9.262	44.518	14.939		51.92	W
ATOM	1288	OH2	TIP		137	12.139	53.137	17.554		56.22	W
ATOM	1289	OH2	TIP	W	138	14.403	57.453	15.838		66.72	M
ATOM	1290	OH2	TIP	W	139	11.017	71.423	23.035		71.76	W
ATOM	1291	OH2	TIP	W	140	10.451	75.718	24.795		58.85	W
ATOM	1292	OH2	TIP	W	141	11.223	65.048	21.172		84.46	W
ATOM	1293	OH2	TIP	W	142	8.196	70.691	21.387		66.14	M
MOTA	1294	OH2	TIP		143	3.381	51.168	17.717	1.00	51.91	W
ATOM	1295	OH2	TIP		144	13.735	48.059	19.325	1.00	73.18	W
ATOM	1296	OH2			145	2.524	42.027	17.393	1.00	80.66	W
MOTA	1297	OH2	TIP		146	2.024	39.150	18.549	1.00	74.07	W
ATOM	1298	OH2	TIP		147	0.486	41.584	19.991	1.00	97.41	W
ATOM	1299	OH2	TIP		148	0.060	40.945	24.577	1.00	78.10	W
		OHO	TIP		149	14.261	36.624	16.034		71.76	W
MOTA	1300	OH2	TIP		150	17.041	33.288	18.134		55.41	W
ATOM	1301					12.012	53.850	23.650		34.32	W
MOTA	1302	OH2	TIP			0.421	41.869	28.444		53.88	W
ATOM	1303	OH2	TIP		152	13.184	36.734	27 569		62.34	I
MOTA	1304	CL-1	بذك	I	1	٠٥.١٥4	20.124	2, 202			
END											

Figure 11V